

1st CAS REACT*search based on  
my interpretation  
of the claims.*

=&gt; d his

(FILE 'HOME' ENTERED AT 12:28:44 ON 17 SEP 2002)

FILE 'HCAPLUS' ENTERED AT 12:28:53 ON 17 SEP 2002

L1 254 S JACQUOT R?/AU  
 L2 1 S L1 AND MIXED ETHER  
 SELECT RN L2 1

FILE 'REGISTRY' ENTERED AT 12:29:25 ON 17 SEP 2002

L3 4 S E1-4

FILE 'HCAPLUS' ENTERED AT 12:29:29 ON 17 SEP 2002

L4 1 S L2 AND L3

*1 citation w/ 4 cpds displayed*

FILE 'CASREACT' ENTERED AT 12:30:18 ON 17 SEP 2002

L5 STR  
 L6 6 S L5  
 L7 STR L5  
 L8 64 S L5 FUL  
 L9 60 S L8/COM *parent set*  
 SAVE L9 REY455CRP/A  
 L10 1 S L7 SSS SAM SUB=L9  
 L11 25 S L7 SSS FUL SUB=L9 *subset 1*  
 SAVE L11 REY455CRS1/A  
 L12 26489 S ALKYLAT?  
 L13 8 S L11 AND L12  
 L14 STR L7  
 L15 1 S L14 SSS SAM SUB=L9  
 L16 21 S L14 SSS FUL SUB=L9 *subset 2*  
 L17 16 S L11 NOT L16  
 L18 1546 S 79-22-1/RRT *methyle chloro formate*  
 L19 12 S L17 NOT L18  
 L20 2 S L19 AND L13  
 L21 6 S L13 NOT L20  
 L22 1 S DIHYDROINDOLES AND L21  
 L23 13 S L19 OR L22 *13 cites*  
 L24 1 S 134:266094/AN *← appl. cite in casreact*  
 L25 0 S L24 AND L23  
 L26 0 S L24 AND L9

FILE 'STNGUIDE' ENTERED AT 13:15:24 ON 17 SEP 2002

FILE 'CASREACT' ENTERED AT 14:15:43 ON 17 SEP 2002

SAVE L16 REY455S2/A TEMP

=&gt; d que 123

L5

STR

*parent rxn*

RRT

*reactant*

PRO

*product*

$$\begin{array}{ccccccc} \text{Cy} & - & \text{C} & - & \text{O} & - & \text{Ak} & - & \text{C} \equiv \text{C} & - & \text{H} \\ 1 & & 2 & & 3 & & 4 & & 5 & & 6 & & 7 \end{array}$$

$$\begin{array}{cccccccc} \text{Cy} & - & \text{C} & - & \text{O} & - & \text{Ak} & - & \text{C} \equiv \text{C} & - & \text{Ak} \\ 8 & & 9 & & 10 & & 11 & & 12 & & 13 & & 14 \end{array}$$

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 4

CONNECT IS E2 RC AT 11

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L7

STR

*subset 1*

RRT

RRT

PRO

$$\begin{array}{ccccccc} \text{Cy} & - & \text{C} & - & \text{O} & - & \text{Ak} & - & \text{C} \equiv \text{C} & - & \text{H} \\ 1 & & 2 & & 3 & & 4 & & 5 & & 6 & & 7 \end{array}$$

$$\begin{array}{cc} \text{Ak} & \sim \text{G1} \\ 15 & 16 \end{array}$$

$$\begin{array}{cccccccc} \text{Cy} & - & \text{C} & - & \text{O} & - & \text{Ak} & - & \text{C} \equiv \text{C} & - & \text{Ak} \\ 8 & & 9 & & 10 & & 11 & & 12 & & 13 & & 14 \end{array}$$

$$\begin{array}{c} \text{O} \\ | \\ \text{O} \sim \text{S} \sim \text{O} \\ @17 \quad 18 \quad 19 \end{array}$$
*halogen**alkylating agent*

VAR G1=X/17

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 4

CONNECT IS E2 RC AT 11

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L8 64 SEA FILE=CASREACT SSS FUL L5 ( 264 REACTIONS)

L9 60 SEA FILE=CASREACT ABB=ON PLU=ON L8/COM

L11 25 SEA FILE=CASREACT SUB=L9 SSS FUL L7 ( 80 REACTIONS)

L12 26489 SEA FILE=CASREACT ABB=ON PLU=ON ALKYLAT?

L13 8 SEA FILE=CASREACT ABB=ON PLU=ON L11 AND L12

L14 STR

*subset 2*

RRT

RRT

PRO

$$\begin{array}{ccccccc} \text{Cy} & - & \text{C} & - & \text{O} & - & \text{Ak} & - & \text{C} \equiv \text{C} & - & \text{H} \\ 1 & & 2 & & 3 & & 4 & & 5 & & 6 & & 7 \end{array}$$

$$\begin{array}{ccc} \text{Ak} & \sim & \text{C} \equiv \text{O} \\ 15 & 16 & 21 \end{array}$$

$$\begin{array}{cccccccc} \text{Cy} & - & \text{C} & - & \text{O} & - & \text{Ak} & - & \text{C} \equiv \text{C} & - & \text{Ak} \\ 8 & & 9 & & 10 & & 11 & & 12 & & 13 & & 14 \end{array}$$

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 4

CONNECT IS E2 RC AT 11

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

*getting rid of alkylating agents*

GRAPH ATTRIBUTES:  
RING(S) ARE ISOLATED OR EMBEDDED  
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE

L16	21	SEA	FILE=CASREACT	SUB=L9	SSS FUL	L14 ( 71 REACTIONS)
L17	16	SEA	FILE=CASREACT	ABB=ON	PLU=ON	L11 NOT L16
L18	1546	SEA	FILE=CASREACT	ABB=ON	PLU=ON	79-22-1/RRT
L19	12	SEA	FILE=CASREACT	ABB=ON	PLU=ON	L17 NOT L18
L20	2	SEA	FILE=CASREACT	ABB=ON	PLU=ON	L19 AND L13
L21	6	SEA	FILE=CASREACT	ABB=ON	PLU=ON	L13 NOT L20
L22	1	SEA	FILE=CASREACT	ABB=ON	PLU=ON	DIHYDROINDOLES AND L21
L23	13	SEA	FILE=CASREACT	ABB=ON	PLU=ON	L19 OR L22

=&gt; d ibib abs fcrdref 1-13

L23 ANSWER 1 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 130:110316 CASREACT

TITLE: Synthesis and characterization of a protected amino alcohol containing ortho-carborane

AUTHOR(S): Wu, Ye; Carroll, Patrick J.; Quintana, William

CORPORATE SOURCE: Dep. Chemistry and Biochemistry, New Mexico State University, Las Cruces, NM, 88003-8001, USA

SOURCE: Polyhedron (1998), 17(19), 3391-3407

CODEN: PLYHDE; ISSN: 0277-5387

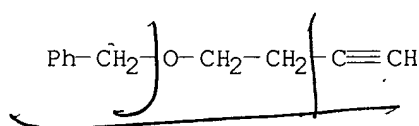
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

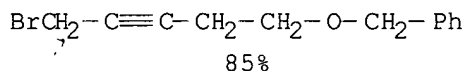
LANGUAGE: English

AB The reaction between the alkyne, N-(5-Benzyloxy-2-pentynyl)phthalimide and decaborane(14) in the presence of di-Me sulfide resulted in the isolation of 1-C<sub>6</sub>H<sub>4</sub>(CO)<sub>2</sub>NCH<sub>2</sub>-2-C<sub>6</sub>H<sub>5</sub>CH<sub>2</sub>OCH<sub>2</sub>CH<sub>2</sub>-1, 2-C<sub>2</sub>B<sub>10</sub>H<sub>10</sub> (5), 1-methylphthalimido-2-ethylbenzyl ether-o-carborane, in moderate yield. Compd. 5 was characterized by single crystal x-ray diffraction study. Compd. 5 crystallizes in the P<sub>2</sub>1<sub>2</sub>1 space group, a = 10.5328 (5) .ANG., b = 11.9209 (6) .ANG., c = 10.3451 (3) .ANG., .alpha. = 110.492 (3).degree., .beta. = 102.868 (3).degree., .gamma. = 87.279 (2).degree., Z = 2, D<sub>calc</sub> = 1.226 g/cm<sup>3</sup>, R = 0.0491 for 3521 reflections with F<sub>o</sub>>4.0.sigma.. Deprotection of the ether linkage of 5 results in the formation of 1-C<sub>6</sub>H<sub>4</sub>(CO)<sub>2</sub>NCH<sub>2</sub>-2-HOCH<sub>2</sub>CH<sub>2</sub>-1, 2-C<sub>2</sub>B<sub>10</sub>H<sub>10</sub> (6), 1-methylphthalimido-2-ethylalc.-o-carborane. The transformation is accomplished by hydrogenation of 5 over a Pd/C catalyst and resulted in the efficient conversion of 5 into 6 (83% yield). Exptl. details and anal. data leading to the identification of the reported compds. is provided.

RX(8) OF 21 - 2 STEPS



1.1. BuLi, THF,  
Cyclohexane  
1.2. HCHO  
2. R:219756-79-3,  
MeCN



REF: Polyhedron, 17(19), 3391-3407; 1998

REFERENCE COUNT: 45 THERE ARE 45 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L23 ANSWER 2 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 128:140989 CASREACT

TITLE: Catalytic Asymmetric Syntheses of Antifungal Sphingofungins and Their Biological Activity as Potent Inhibitors of Serine Palmitoyltransferase (SPT)

AUTHOR(S): Kobayashi, Shu; Furuta, Takayuki; Hayashi, Takaomi; Nishijima, Masahiro; Hanada, Kentaro

CORPORATE SOURCE: Department of Applied Chemistry Faculty of Science,

Searched by Susan Hanley 305-4053

Page 1

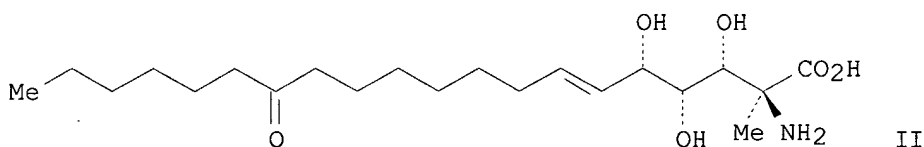
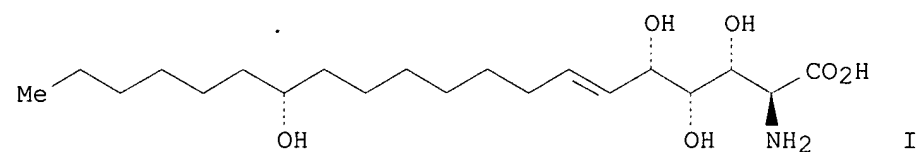
SOURCE: Science University of Tokyo (SUT), Tokyo, 162, Japan  
Journal of the American Chemical Society (1998),  
120(5), 908-919  
CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

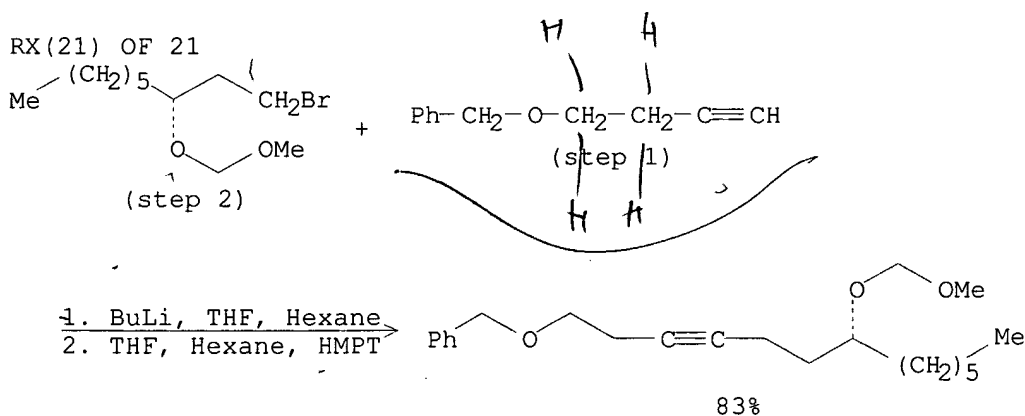
DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Unambiguous synthetic routes to sphingofungins B (I) and F (II) and to their stereoisomers have been developed based on the tin(II)-catalyzed asym. aldol reaction (Chiral Lewis Acid-Controlled Synthesis (CLAC Synthesis)). Efficient enantioselective synthesis using a catalytic amt. of a chiral source as well as the effectiveness of this strategy for the synthesis of the sphingofungin family have been successfully demonstrated. Using the stereoisomers of sphingofungin B synthesized, the relevance of its stereochem. to its serine palmitoyltransferase inhibitory activity has been revealed.



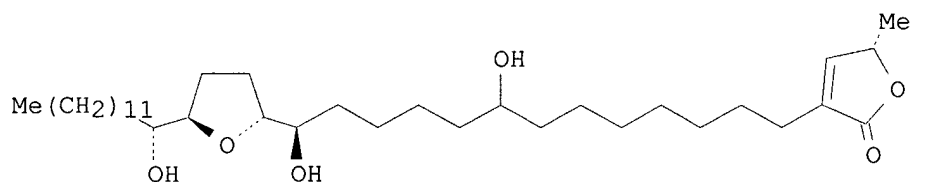
REF: Journal of the American Chemical Society, 120(5), 908-919; 1998

L23 ANSWER 3 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 126:31210 CASREACT

TITLE: Synthetic studies on Annonaceous acetogenins. VII.  
Total synthesis of (8'R)- and (8'S)-corossolin

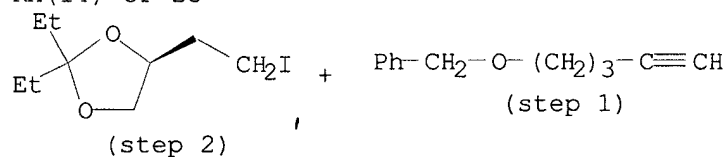
AUTHOR(S): Makabe, Hidefumi; Tanimoto, Hisahide; Tanaka, Akira; Oritani, Takayuki  
 CORPORATE SOURCE: Dep. Applied Biological Chemistry Faculty Agriculture, Graduate School Agriculture, Tohoku Univ., Sendai, 981, Japan  
 SOURCE: Heterocycles (1996), 43(10), 2229-2248  
 CODEN: HTCYAM; ISSN: 0385-5414  
 PUBLISHER: Japan Institute of Heterocyclic Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



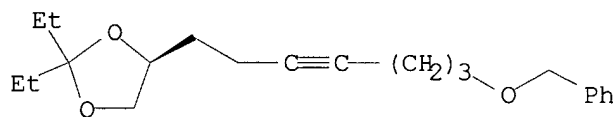
I

AB A convergent stereoselective total synthesis of (8'R)- and (8'S)-corossolin (I) has been performed via a multi-step process. Comparison of the mp,  $[\alpha]_D$ , IR and NMR data of both synthetic materials with those reported for natural I did not allow for the strict detn. of the configuration at the C-8' hydroxyl group of I. However, a slight chem. shift difference at the C-8' methine proton was obsd. in the 1H-NMR spectra of the corresponding tris-MTPA esters of synthetic (8'R)- and (8'S)-I, indicating that if the tris-MTPA ester of natural I is available, the stereochem. at the C-8' hydroxyl group of corossolin will be established.

RX(14) OF 23



1. BuLi, THF, Hexane  
 2. HMPT



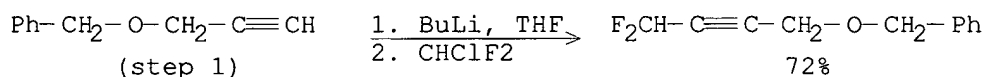
59%

REF: Heterocycles, 43(10), 2229-2248; 1996

L23 ANSWER 4 OF 13 CASREACT COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 126:7656 CASREACT  
 TITLE: Novel synthesis and application of  $\gamma$ -difluoromethylated prop-2-ynyl and allylic

alcohols  
 AUTHOR(S): Konno, Tsutomu; Kitazume, Tomoya  
 CORPORATE SOURCE: Dep. Bioeng., Tokyo Inst. Technol., Yokohama, 226, Japan  
 SOURCE: Chemical Communications (Cambridge) (1996), (19), 2227-2228  
 CODEN: CHCOFS; ISSN: 1359-7345  
 PUBLISHER: Royal Society of Chemistry  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB The reaction of chlorodifluoromethane with various acetylides derived from the corresponding prop-2-ynyl alcs. proceeds smoothly to afford difluoromethylated compds., e.g.,  $\text{Me}(\text{CH}_2)_4\text{CH}(\text{OSiMe}_2\text{CMe}_3)\text{C.tplbond.CCF}_2$ , in high yields; synthetic applications of the materials are also given.

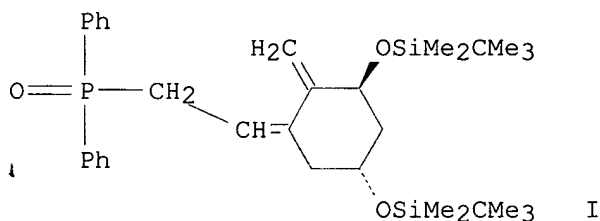
RX(1) OF 3



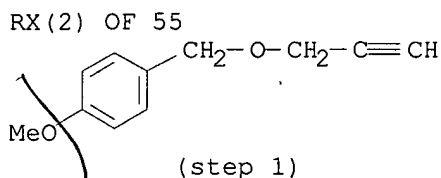
REF: Chemical Communications (Cambridge), (19), 2227-2228; 1996

L23 ANSWER 5 OF 13 CASREACT COPYRIGHT 2002 ACS

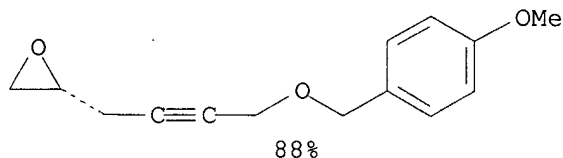
ACCESSION NUMBER: 122:240140 CASREACT  
 TITLE: An efficient route to a key A-ring synthon for 1.alpha.,25-dihydroxyvitamin D3 and its analogs  
 AUTHOR(S): Hatakeyama, Susumi; Irie, Hiroshi; Shintani, Takashi; Noguchi, Yohko; Yamada, Hidetoshi; Nishizawa, Mugio  
 CORPORATE SOURCE: Fac. of Pharmaceutical Sciences, Nagasaki Univ., Nagasaki, 852, Japan  
 SOURCE: Tetrahedron (1994), 50(47), 13369-76  
 CODEN: TETRAB; ISSN: 0040-4020  
 PUBLISHER: Elsevier  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB An efficient and highly stereoselective route to the Roche A-ring synthon I for 1.alpha.,25-dihydroxyvitamin D3 from R-(-)-epichlorohydrin has been developed utilizing double propargylation of R-(-)-epichlorohydrin and palladium(0)-catalyzed intramol. Heck type of reaction of an .omega.-vinyl-(Z)-iodoalkene as key steps.

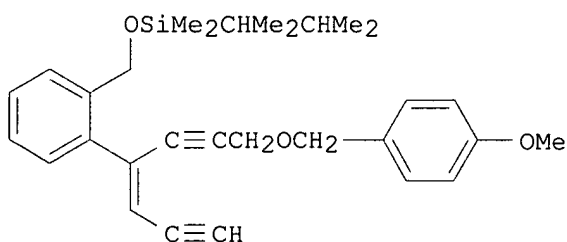


1. Epichlorohydrin,  
BuLi, BF<sub>3</sub>-Et<sub>2</sub>O,  
THF  
2. NaH, THF



REF: Tetrahedron, 50(47), 13369-76; 1994  
NOTE: KEY STEP

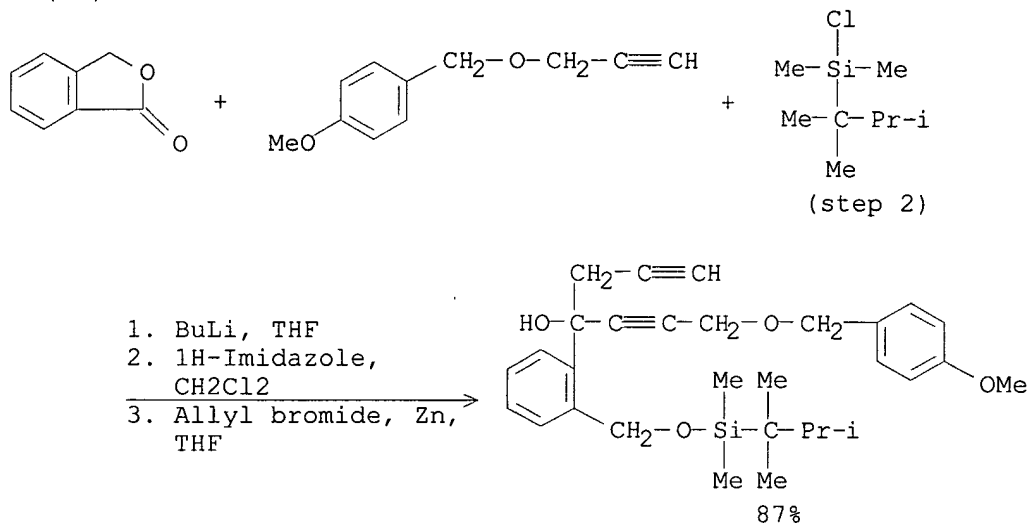
L23 ANSWER 6 OF 13 CASREACT COPYRIGHT 2002 ACS  
ACCESSION NUMBER: 122:213682 CASREACT  
TITLE: A convenient synthesis of aryl conjugated enediynes  
AUTHOR(S): Shibuya, Masayuki; Sakai, Yasuhiro; Naoe, Yoshimitsu  
CORPORATE SOURCE: Fac. Pharm. Sci., Univ. Tokushima, Tokushima, 770, Japan  
SOURCE: Tetrahedron Letters (1995), 36(6), 897-8  
CODEN: TELEAY; ISSN: 0040-4039  
PUBLISHER: Elsevier  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Novel synthetic method for acyclic cis-hex-3-ene-1,5-diyne derivs. via elimination of tert-hydroxy group has been described. 3-(4-Methoxybenzyloxy)propyne was treated with NuLi followed by phthalide to give the appropriate hydroxy deriv. which was protected, the product condensed with propargyl bromide to give the tert-alc. which was treated with mesyl chloride and NEt<sub>3</sub> to give the title E- and Z-I.



RX(22) OF 30 - 3 STEPS



REF: Tetrahedron Letters, 36(6), 897-8; 1995

L23 ANSWER 7 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 115:28777 CASREACT

TITLE: Palladium-catalyzed coupling reactions of trifluoroacetimidoyl iodides with olefins and 1-alkynes

AUTHOR(S): Uneyama, Kenji; Watanabe, Hisayuki

CORPORATE SOURCE: Fac. Eng., Okayama Univ., Okayama, 700, Japan

SOURCE: Tetrahedron Lett. (1991), 32(11), 1459-62

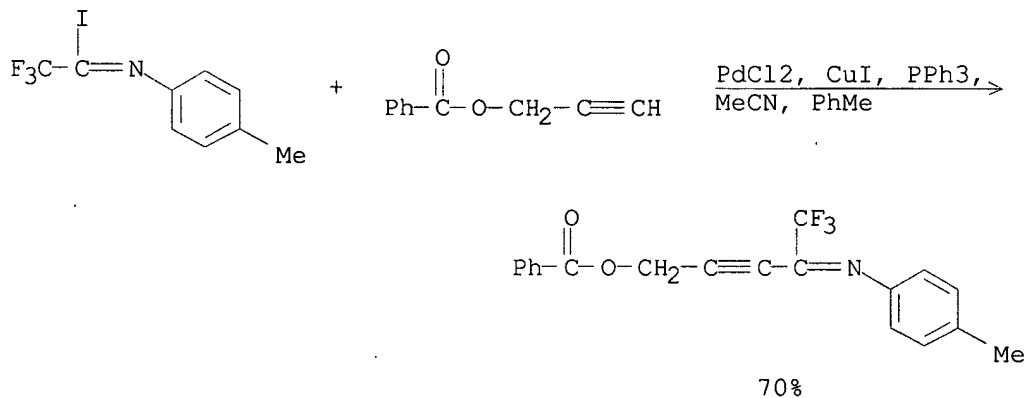
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

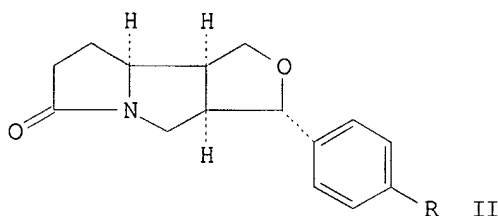
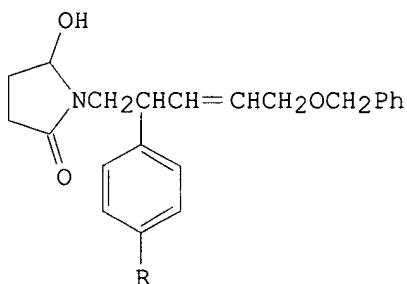
AB Palladium-catalyzed coupling of trifluoroacetimidoyl iodides with olefins and 1-alkynes affords trifluoromethylated .alpha.,.beta.-unsatd. imines e.g. MeO<sub>2</sub>CCH:CHC(CF<sub>3</sub>):NC<sub>6</sub>H<sub>4</sub>Me-p, which are transformed into nitrogen heterocycles bearing CF<sub>3</sub>-group.

RX(1) OF 4



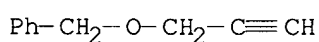
REF: Tetrahedron Lett., 32(11), 1459-62; 1991

L23 ANSWER 8 OF 13 CASREACT COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 113:58984 CASREACT  
 TITLE: N-Acyliminium cyclizations: formation of the furo[3,4-a]pyrrolizine ring system  
 AUTHOR(S): Ent, Hugo; De Koning, Henk; Speckamp, W. Nico  
 CORPORATE SOURCE: Lab. Org. Chem., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.  
 SOURCE: Heterocycles (1990), 30(1, Spec. Issue), 501-5  
 CODEN: HTCYAM; ISSN: 0385-5414  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



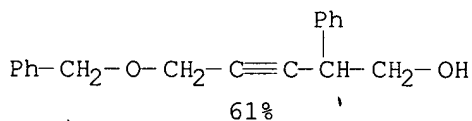
AB Hydroxylactams I (R = H, MeO) upon treatment with HCO<sub>2</sub>H were converted to the title compds. II in 44-67% yield via the 2-aza-Cope rearrangement cyclization of the N-acyliminium ions. The prepn. of I is also described.

RX(1) OF 20



Styrene oxide, Mg, EtBr, Et<sub>2</sub>O

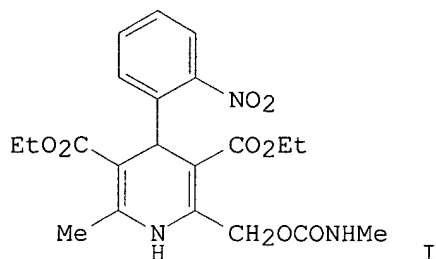
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REF: Heterocycles, 30(1, Spec. Issue), 501-5; 1990

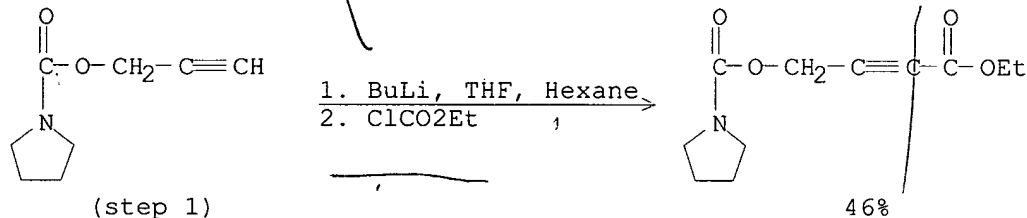
L23 ANSWER 9 OF 13 CASREACT COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 111:194537 CASREACT  
 TITLE: An improved synthesis of 2-[(carbamoyloxy)methyl]-1,4-dihydropyridine  
 AUTHOR(S): Suzuki, Kunio; Ushijima, Ryosuke; Miyano, Tetsuji; Nakagawa, Susumu  
 CORPORATE SOURCE: Okazaki Res. Lab., Banyu Pharm. Co., Ltd., Okazaki, 444, Japan  
 SOURCE: Heterocycles (1989), 29(3), 497-509  
 CODEN: HTCYAM; ISSN: 0385-5414  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

GI



AB A synthesis of 3-amino-4-carbamoyloxybutenoic esters by conjugate addn. of  $\text{NH}_3$  to 4-carbamoyloxy-2-butynoic esters is reported. Numerous dihydropyridines were prepd. from the resulting 3-aminobutenoates by cyclocondensation with benzylideneacetoacetates. Thus,  $\text{MeNHCO}_2\text{CH}_2\text{C}(\text{t})\text{CO}_2\text{Et}$  was treated with  $\text{AcONH}_4$  in  $\text{MeOH}$  at  $60^\circ$  to give 44%  $\text{MeNHCO}_2\text{CH}_2\text{C}(\text{NH}_2):\text{CHCO}_2\text{Et}$  which was treated with  $2\text{-O}_2\text{NC}_6\text{H}_4\text{CH}:\text{C}(\text{CO}_2\text{Et})\text{COMe}$  in  $\text{EtOH}$  to give 43% the dihydropyridine I.

RX(61) OF 173



REF: Heterocycles, 29(3), 497-509; 1989

L23 ANSWER 10 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 111:153582 CASREACT

TITLE: Long-acting dihydropyridine calcium antagonists. 3. Synthesis and structure-activity relationships for a series of 2-[(heterocyclylmethoxy)methyl] derivatives

AUTHOR(S): Alker, David; Campbell, Simon F.; Cross, Peter E.; Burges, Roger A.; Carter, Anthony J.; Gardiner, Donald G.

CORPORATE SOURCE: Pfizer Cent. Res., Sandwich/Kent, CT13 9NJ, UK

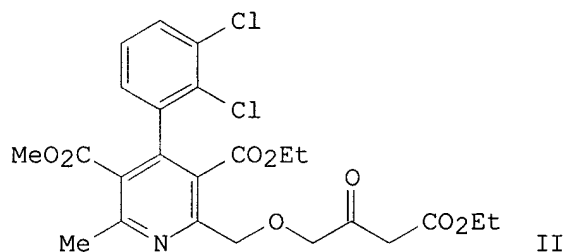
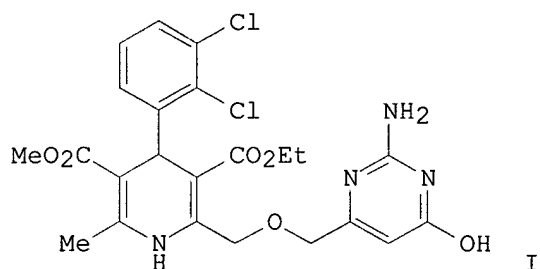
SOURCE: J. Med. Chem. (1989), 32(10), 2381-8

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

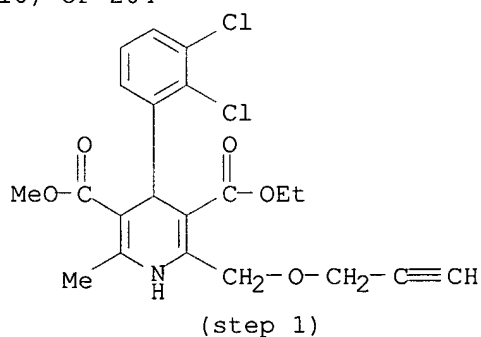
LANGUAGE: English

GI



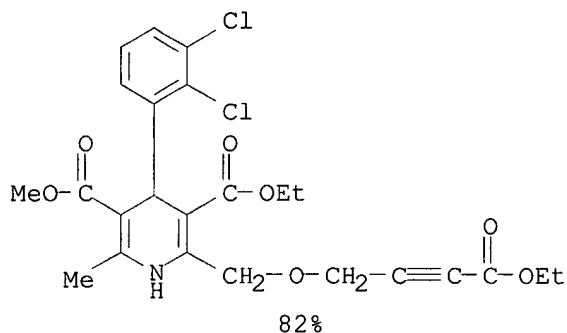
AB Title compds., e.g. I, were prepd. and some of the compds. were identified by  $^1\text{H}$  NMR. Thus, I was prepd. from  $\text{H}_2\text{NCMe:CHCO}_2\text{Me}$  via cyclization of ester II with  $\text{HN:C(NH}_2)_2$ . The Ca antagonist activity of the compds. on rat aorta is compared with the neg. inotropic potency in a Langendorff model. Several compds. are more potent than nifedipine and show greater selectivity for the vasculature over the heart. I was identified as a potent ( $\text{ED}_{50} = 1.6 \text{ } \mu\text{M}$ ), tissue-selective Ca antagonist which proved to have a markedly longer duration of action ( $>4.5 \text{ h}$ ) than nifedipine i. v. in dogs.

RX(10) OF 204



1. BuLi,  $\text{CO}_2$ , THF  
 2. EtBr,  $\text{PhCH}_2\text{NMe}_3^+\text{OH}^-$ ,  
 DMSO

RX(10) OF 204



REF: J. Med. Chem., 32(10), 2381-8; 1989

L23 ANSWER 11 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER:

108:75216 CASREACT /

TITLE:

Stereocontrolled formation of 1,2-dihydroindoles

AUTHOR(S):

Veenstra, S. J.; Fortgens, H. P.; Vijn, R. J.; De Jong, B. S.; Speckamp, W. N.

CORPORATE SOURCE:

Lab. Org. Chem., Univ. Amsterdam, Amsterdam, 1018 WS, Neth.

SOURCE:

Tetrahedron (1987), 43(6), 1147-56

CODEN: TETRAB; ISSN: 0040-4020

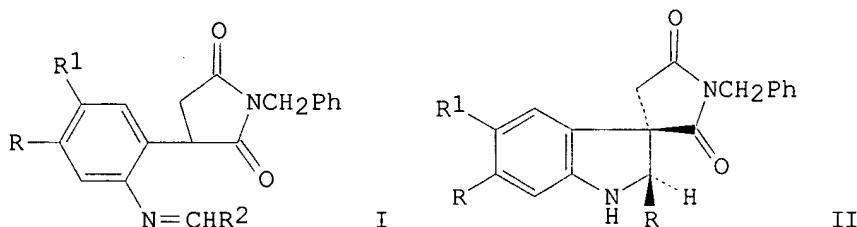
DOCUMENT TYPE:

Journal

LANGUAGE:

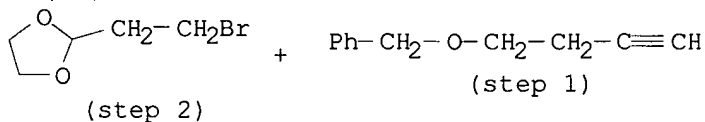
English

GI

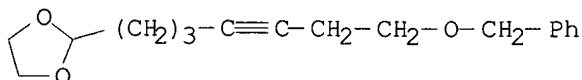


AB Stereoselective cyclization of imines I [R = R1 = H, R2 = Ph, 4-R3C6H4, 3-pyridyl, (E)-PhCH:CH, Pr, Me3C, PhCH2O(CH2)2C.tplbond.C(CH2)2, 2-(ethylenedioxy)propyl; R3 = MeO, O2N, NC; R = H, R1 = Cl, R2 = Ph; R = MeO, R1 = H, R2 = Ph] in the presence of NaOCMe3 gave cis-spiroindolines II in 47-83% yields. Cyclization with less bulky alkoxides NaOEt or NaOMe gave trans-II in 20-90% yields. With electron rich imines, the cyclization occurs thermally. Lewis acid catalyst also cause cyclization of I to cis-II, but the reaction is less stereoselective.

RX(49) OF 182



1. Li, Fe(NO<sub>3</sub>)<sub>3</sub>, NH<sub>3</sub>,  
DMSO  
2. NH<sub>3</sub>, DMSO



REF: Tetrahedron, 43(6), 1147-56; 1987

L23 ANSWER 12 OF 13 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 107:6730 CASREACT

TITLE: Alkylation of stabilized acetylides in DMSO.  
Preparation of .alpha.,.beta.-acetylenic alcohols and acetals

AUTHOR(S): Chong, J. Michael; Wong, Susanna

CORPORATE SOURCE: Guelph-Waterloo Cent. Grad. Work Chem., Univ.  
Waterloo, Waterloo, ON, N2L 3G1, Can.

SOURCE: Tetrahedron Lett. (1986), 27(45), 5445-8

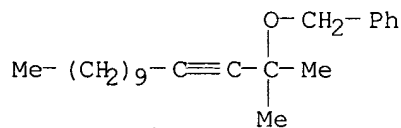
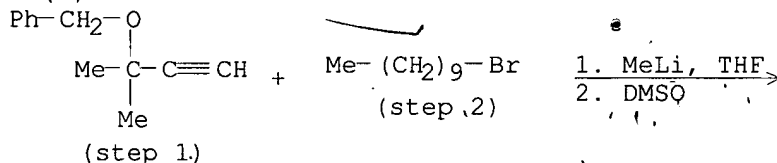
CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Lithiation of stabilized RC.tplbond.CH [I, R = CH<sub>2</sub>OTHP (THP = 2-tetrahydropyranyl), Ph, CH(OEt)<sub>2</sub>] with MeLi in DMSO, followed by alkylation with R<sub>1</sub>Br [R<sub>1</sub> = Me(CH<sub>2</sub>)<sub>9</sub>, Me(CH<sub>2</sub>)<sub>5</sub>, Me<sub>2</sub>CHCH<sub>2</sub>] gave disubstituted alkynes RC.tplbond.CR<sub>1</sub> in 42-87% yields. Unstabilized I [R = (CH<sub>2</sub>)<sub>2</sub>OTHP, Me(CH<sub>2</sub>)<sub>5</sub>] gave products resulting from alkylation of the solvent. Thus, THPOCH<sub>2</sub>C.tplbond.CH was alkylated with Me(CH<sub>2</sub>)<sub>9</sub>Br to give 87% THPOCH<sub>2</sub>C.tplbond.C(CH<sub>2</sub>)<sub>9</sub>Me, which was deprotected and reduced to either (E)- or (Z)-Me(CH<sub>2</sub>)<sub>9</sub>CH:CH<sub>2</sub>OH in 91 or 96% yield.

RX(2) OF 26



76%

REF: Tetrahedron Lett., 27(45), 5445-8; 1986

L23 ANSWER 13 OF 13 CASREACT COPYRIGHT 2002 ACS

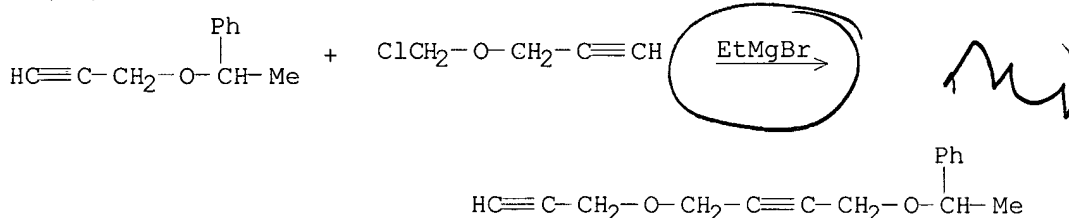
ACCESSION NUMBER: 93:167775 CASREACT

TITLE: Propargyl ether of .alpha.-phenylethyl alcohol and its

AUTHOR(S): Karayev, S. F.; Dzhaferov, D. S.; Askerov, M. E.  
 CORPORATE SOURCE: Azerb. Inst. Nefti Khim., Baku, USSR  
 SOURCE: Zh. Org. Khim. (1980), 16(5), 928-33  
 CODEN: ZORKAE; ISSN: 0514-7492  
 DOCUMENT TYPE: Journal  
 LANGUAGE: Russian

AB PhMgBr reacted with ClCHMeOCH<sub>2</sub>C.tplbond.CH in refluxing Et<sub>2</sub>O to give 38% PhCHMeOCH<sub>2</sub>C.tplbond.CH (I) and 15% PhCHMeCl. I reacted with H<sub>2</sub>O contg. HgO-H<sub>2</sub>SO<sub>4</sub> at 60.degree., HOCH<sub>2</sub>CH<sub>2</sub>OH contg. HgO and BF<sub>3</sub>.OEt<sub>2</sub>, R<sub>2</sub>R<sub>1</sub>SiH (R = R<sub>1</sub> = EtO; R = Bu, R<sub>1</sub> = Me), and HCHO-R<sub>2</sub>NH (R<sub>2</sub>N = Et<sub>2</sub>N, piperidino, morpholino) in the presence of Cu<sub>2</sub>Cl<sub>2</sub> to give 54% PhCHMeOCH<sub>2</sub>COMe (II), 69% II ethylene ketal, 54-6% PhCHMeOCH<sub>2</sub>CH:CHSiR<sub>2</sub>R<sub>1</sub> (same R, R<sub>1</sub>) and 64-8% PhCHMeOCH<sub>2</sub>C.tplbond.CR<sub>2</sub> (III; R<sub>2</sub> = CH<sub>2</sub>NR<sub>2</sub>, same NR<sub>2</sub>), resp. I reacted with EtMgBr to give III (R<sub>2</sub> = MgBr), which reacted with Me<sub>2</sub>CO, Me<sub>3</sub>SiCl, MeEtSiHCl and ClCH<sub>2</sub>OCH<sub>2</sub>C.tplbond.CH (IV) to give 46-61% III [R<sub>2</sub> = CMe<sub>2</sub>OH (V), SiMe<sub>3</sub>, SiHMeEt (VI), CH<sub>2</sub>OCH<sub>2</sub>C.tplbond.CH, resp.]. IV and V reacted to give 45% III (R<sub>2</sub> = CMe<sub>2</sub>OCH<sub>2</sub>OCH<sub>2</sub>C.tplbond.CH). VI added to HC.tplbond.CH<sub>2</sub>OH to give 44% III (R<sub>2</sub> = SiMeEtCH:CHCH<sub>2</sub>OH).

RX(12) OF 22



REF: Zh. Org. Khim., 16(5), 928-33; 1980

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L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 2001:247298 HCAPLUS  
 DOCUMENT NUMBER: 134:266094  
 TITLE: Method for preparing substituted mixed alkynyl ethers  
 INVENTOR(S): **Jacquot, Roland**  
 PATENT ASSIGNEE(S): Rhodia Chimie, Fr.  
 SOURCE: PCT Int. Appl., 26 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023338	A1	20010405	WO 2000-FR2704	20000929
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
FR 2798928	A1	20010330	FR 1999-12146	19990929
EP 1216220	A1	20020626	EP 2000-966235	20000929
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				

PRIORITY APPLN. INFO.: FR 1999-12146 A 19990929  
 WO 2000-FR2704 W 20000929

OTHER SOURCE(S): CASREACT 134:266094; MARPAT 134:266094

AB The invention concerns a method for prepg. substituted mixed alkynyl ethers. More particularly, the invention concerns the prepn. of **mixed ethers** derived from a substituted benzyl alc. and an alkynyl alc. The inventive method for prepg. a substituted mixed benzyl/alkynyl ether from a mixed benzyl/alkynyl ether having a hydrogen atom on the triple bond is characterized in that it consists in reacting a **mixed ether** derived from a benzyl alc. and an alkynyl alc. having a hydrogen atom on the triple bond with an alkylating agent, in the presence of a neg. ion chem. ionizing reagent. E.g., methylation of [1-(prop-1-ynyloxy)ethyl]-3,4-dimethoxybenzene, prepd. by reaction of 1-[3,4-dimethoxyphenyl]ethan-1-ol with propargyl alc. in presence of HY zeolite, with Me sulfate gave [1-(but-2-ynyloxy)ethyl]-3,4-dimethoxybenzene.

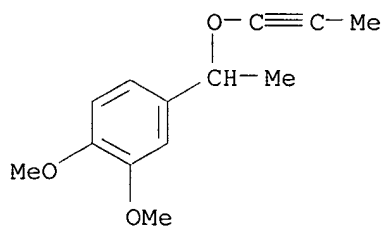
IT **332112-39-7P**

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (prepn. of mixed alkynyl ethers)

RN 332112-39-7 HCAPLUS

CN Benzene, 1,2-dimethoxy-4-[1-(1-propynyloxy)ethyl]- (9CI) (CA INDEX NAME)



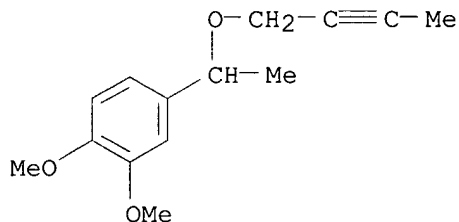


IT 185676-84-0P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
(Preparation)  
(prepn. of mixed alkynyl ethers)

RN 185676-84-0 HCAPLUS

CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)

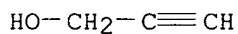


IT 107-19-7, Propargyl alcohol 5653-65-6

RL: RCT (Reactant); RACT (Reactant or reagent)  
(prepn. of mixed alkynyl ethers)

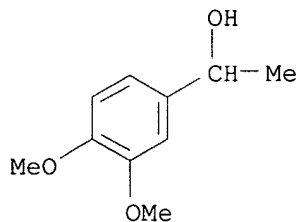
RN 107-19-7 HCAPLUS

CN 2-Propyn-1-ol (8CI, 9CI) (CA INDEX NAME)



RN 5653-65-6 HCAPLUS

CN Benzenemethanol, 3,4-dimethoxy-.alpha.-methyl- (9CI) (CA INDEX NAME)



IC ICM C07C043-215

ICS C07C041-30

CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

ST alkynyl ether prepn

IT Zeolite HY

RL: CAT (Catalyst use); USES (Uses)  
(prepn. of mixed alkynyl ethers)

IT Ethers, preparation  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (prepn. of mixed alkynyl ethers)

IT **332112-39-7P**  
 RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic  
 preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. of mixed alkynyl ethers)

IT **185676-84-0P**  
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (prepn. of mixed alkynyl ethers)

IT **107-19-7, Propargyl alcohol 5653-65-6**  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (prepn. of mixed alkynyl ethers)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

Reg/HCAPLUS SEARCH Based on Appl's

REYES 10/088,455

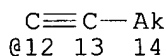
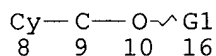
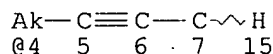
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VAR G1=4/12

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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

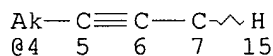
STEREO ATTRIBUTES: NONE

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L3 ( 2197)SEA FILE=REGISTRY ABB=ON PLU=ON L2/COM

L4 STR

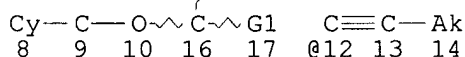
product search



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VAR G1=4/12

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 4

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L5 2046 SEA FILE=REGISTRY SUB=L3 SSS FUL L4

L33 647 SEA FILE=HCAPLUS ABB=ON PLU=ON L5/PREP

L50 3884 SEA FILE=HCAPLUS ABB=ON PLU=ON ETHERS, PREPARATION/CT

L52 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 AND L33

L58 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L52 AND (?ALKYN? OR ?ACETYLEN?)

)

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L58 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:677340 HCAPLUS

DOCUMENT NUMBER: 135:371267

TITLE: Double Cationic Propargylation: From Linear to Polycyclic Ethers

AUTHOR(S): Diaz, David; Martin, Tomas; Martin, Victor S.

CORPORATE SOURCE: Instituto Universitario de Bio-Organica "Antonio Gonzalez", Universidad de La Laguna, La Laguna Tenerife, 38206, Spain

SOURCE: Organic Letters (2001), 3(21), 3289-3291

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The trapping of cations generated from  $\text{Co}_2(\text{CO})_6$ -bispropargylic alcs. provided diethers in good yield. The procedure is also valid when two vicinal **acetylenes** are present. The methodol. can be applied to the synthesis of sym. or unsym. linear or cyclic propargylic ethers. The use of substrates with a stereochem. defined secondary nucleophilic alc. provided cyclic ethers with a high degree of stereocontrol.

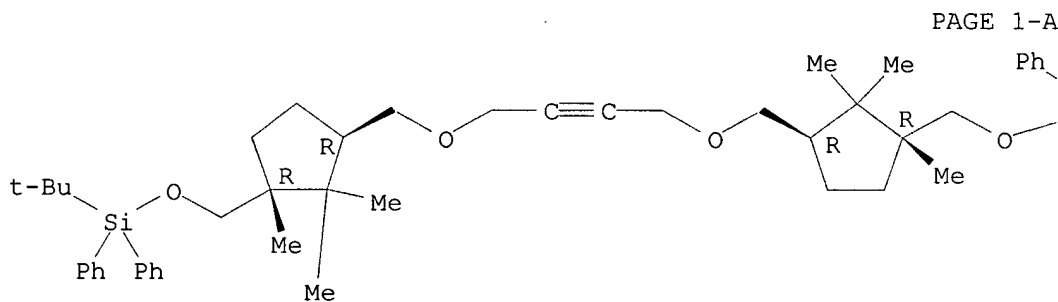
IT 374077-45-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of dipropargylic ethers form propargylic alcs.)

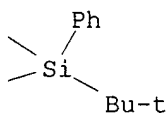
RN 374077-45-9 HCAPLUS

CN Silane, [2-butyne-1,4-diylbis[oxymethylene[(1R,3R)-1,2,2-trimethyl-3,1-cyclopentanediy]methyleneoxy]]bis[(1,1-dimethylethyl)diphenyl-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.



PAGE 1-B



REFERENCE COUNT:

15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L58 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:247298 HCAPLUS

DOCUMENT NUMBER: 134:266094

TITLE: Method for preparing substituted mixed **alkynyl** ethers

INVENTOR(S): Jacquot, Roland

PATENT ASSIGNEE(S): Rhodia Chimie, Fr.

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023338	A1	20010405	WO 2000-FR2704	20000929
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG FR 2798928 A1 20010330 FR 1999-12146 19990929 EP 1216220 A1 20020626 EP 2000-966235 20000929 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL PRIORITY APPLN. INFO.: FR 1999-12146 A 19990929 WO 2000-FR2704 W 20000929				

OTHER SOURCE(S): CASREACT 134:266094; MARPAT 134:266094

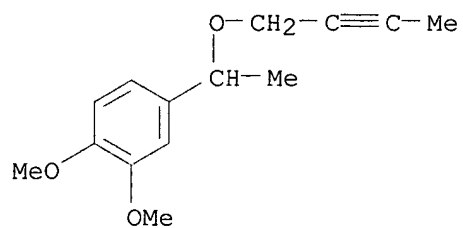
AB The invention concerns a method for prepg. substituted mixed **alkynyl** ethers. More particularly, the invention concerns the prepn. of mixed ethers derived from a substituted benzyl alc. and an **alkynyl** alc. The inventive method for prepg. a substituted mixed benzyl/**alkynyl** ether from a mixed benzyl/**alkynyl** ether having a hydrogen atom on the triple bond is characterized in that it consists in reacting a mixed ether derived from a benzyl alc. and an **alkynyl** alc. having a hydrogen atom on the triple bond with an alkylating agent, in the presence of a neg. ion chem. ionizing reagent. E.g., methylation of [1-(prop-1-ynyloxy)ethyl]-3,4-dimethoxybenzene, prepd. by reaction of 1-[3,4-dimethoxyphenyl]ethan-1-ol with propargyl alc. in presence of HY zeolite, with Me sulfate gave [1-(but-2-ynyloxy)ethyl]-3,4-dimethoxybenzene.

IT 185676-84-0P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP** (Preparation)  
 (prepn. of mixed **alkynyl** ethers)

RN 185676-84-0 HCAPLUS

CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d ibib abs hitstr 3

L58 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:352798 HCAPLUS

DOCUMENT NUMBER: 129:40972

TITLE: Phase-transfer procedure for the preparation of benzyl ethers

INVENTOR(S): Arvai, Geza; Bertok, Bela; Kuruczne, Ribai Zsuzsanna; Pap, Laszlo; Szekely, Istvan

PATENT ASSIGNEE(S): Chinoin Gyogyszer Es Vegyeszeti Termekek Gyara Rt., Hung.; Bertok, Bela; Kuruczne Ribai, Zsuzsanna; Pap, Laszlo; Szekely, Istvan

SOURCE: PCT Int. Appl., 23 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9822417	A1	19980528	WO 1997-HU74	19971112
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9850644	A1	19980610	AU 1998-50644	19971112
ZA 9710317	A	19980610	ZA 1997-10317	19971114
TW 434214	B	20010516	TW 1997-86119822	19971227
PRIORITY APPLN. INFO.:			HU 1996-3178	A 19961118
			WO 1997-HU74	W 19971112

OTHER SOURCE(S): MARPAT 129:40972

AB Mixed ethers Ar(CHR1)nOR2 [Ar = (un)substituted alicyclic, arom. or .gtoreq.1 heteroatom-contg. heterocyclic moiety; R1 = H, C1-4 (halo)alkyl, C2-4 alkenyl, (un)substituted Ph, C3-6 cycloalkyl; R2 = (un)substituted C1-6 alkyl, C3-6 alkenyl, C3-6 **alkynyl**, etc.; n = 1, 2], chem. intermediates or arthropodicide synergists (no data), were prepd. by condensation of compds. Ar(CHR1)nX (I; X = OH, halo, sulfo ester; Ar, R1, n as defined) with compds. R2Y (II; Y = OH, halo, sulfo ester; R2 as defined) where 1 of I, II is an alc. The reaction is carried out under heterogeneous conditions in the presence of an aq. base and a phase transfer catalyst and the resulting product is optionally stabilized by the addn. of a base and/or anti-oxidant. For example, adding 40% aq. KOH and Bu4NBr to a soln. of 2-butyne-1-ol and 1,2-dimethoxy-4-chloromethyl-5-propylbenzene in CH2Cl2 and stirring the whole vigorously for 2 h at ambient temp. gave 90.3% 1-(2-butyneoxyethyl)-3,4-dimethoxy-6-propylbenzene.

IT 185676-84-0P 186086-43-1P 191610-18-1P

208248-76-4P 208248-77-5P 208248-81-1P

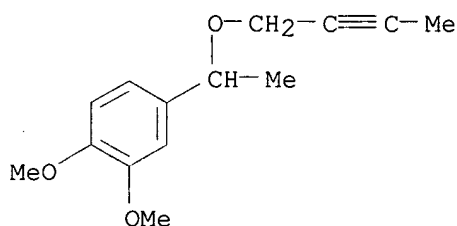
208248-82-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

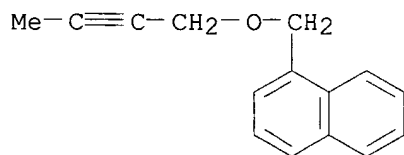
(phase-transfer procedure for the prepn. of benzyl ethers)

RN 185676-84-0 HCAPLUS

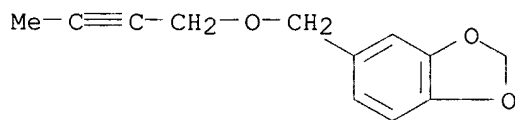
CN Benzene, 4-[1-(2-butyneoxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



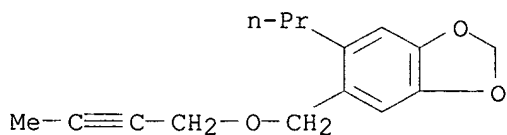
RN 186086-43-1 HCAPLUS  
CN Naphthalene, 1-[(2-butynyloxy)methyl]- (9CI) (CA INDEX NAME)



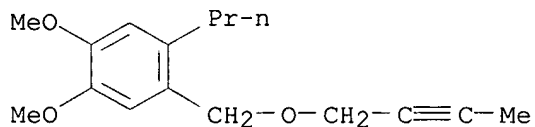
RN 191610-18-1 HCAPLUS  
CN 1,3-Benzodioxole, 5-[(2-butynyloxy)methyl]- (9CI) (CA INDEX NAME)



RN 208248-76-4 HCAPLUS  
CN 1,3-Benzodioxole, 5-[(2-butynyloxy)methyl]-6-propyl- (9CI) (CA INDEX NAME)

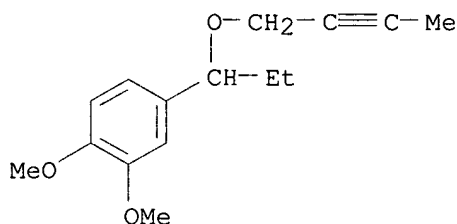


RN 208248-77-5 HCAPLUS  
CN Benzene, 1-[(2-butynyloxy)methyl]-4,5-dimethoxy-2-propyl- (9CI) (CA INDEX NAME)

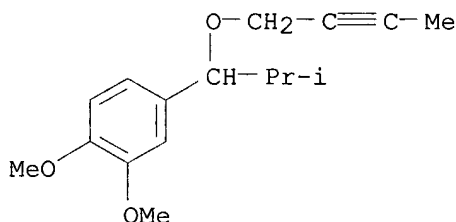


RN 208248-81-1 HCAPLUS  
CN Benzene, 4-[1-(2-butynyloxy)propyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)





RN 208248-82-2 HCAPLUS  
 CN Benzene, 4-[1-(2-butynyloxy)-2-methylpropyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



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L58 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2002 ACS  
 IC ICM C07C041-16  
 ICS C07D317-54; C07C043-215; C07C043-225; C07C043-205  
 CC 25-9 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)  
 ST benzyl ether prepn phase transfer; butynol etherification  
 dimethoxychloromethylpropylbenzene tetrabutylammonium catalyst;  
 chloromethylpropylbenzene etherification butynol tetrabutylammonium  
 catalyst  
 IT **Ethers, preparation**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (mixed; process for the prepn. of benzyl ethers by use of phase  
 transfer)  
 IT Etherification  
 (phase-transfer procedure for the prepn. of benzyl ethers)  
 IT Phase transfer catalysts  
 (process for the prepn. of benzyl ethers by use of phase transfer)  
 IT 93-03-8, Veratryl alcohol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (bromination and etherification of diethylene glycol monobutyl ether;  
 phase-transfer procedure for the prepn. of benzyl ethers)  
 IT 495-76-1, Piperonyl alcohol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (bromination; phase-transfer procedure for the prepn. of benzyl ethers)  
 IT 86-52-2, 1-(Chloromethyl)naphthalene 1938-32-5 54675-73-9  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (etherification of butynol; phase-transfer procedure for the prepn. of  
 benzyl ethers)  
 IT 107-05-1, Allyl chloride 926-57-8, 1,3-Dichloro-2-butene 3355-28-0,  
 1-Bromo-2-butyne  
 RL: RCT (Reactant); RACT (Reactant or reagent)

- (etherification of methylveratryl alc.; phase-transfer procedure for the prepn. of benzyl ethers)
- IT 10548-83-1 67031-41-8  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (etherification with bromobutyne; phase-transfer procedure for the prepn. of benzyl ethers)
- IT 5653-65-6, .alpha.-Methylveratryl alcohol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (etherification with dichlorobutene; phase-transfer procedure for the prepn. of benzyl ethers)
- IT 112-34-5, Diethylene glycol monobutyl ether  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (etherification with veratryl bromide; phase-transfer procedure for the prepn. of benzyl ethers)
- IT 764-01-2, 2-Butyn-1-ol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (etherification; phase-transfer procedure for the prepn. of benzyl ethers)
- IT 311-28-4, Tetrabutylammonium iodide 25316-59-0, Benzyltributylammonium bromide  
 RL: CAT (Catalyst use); USES (Uses)  
 (phase-transfer procedure for the prepn. of benzyl ethers)
- IT 51-03-6P 34827-25-3P **185676-84-0P 186086-43-1P**  
**191610-18-1P 208248-76-4P 208248-77-5P**  
 208248-78-6P 208248-79-7P 208248-80-0P **208248-81-1P**  
**208248-82-2P**  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (phase-transfer procedure for the prepn. of benzyl ethers)
- IT 2606-51-1P, Piperonyl bromide  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (prepn. and etherification with butynol; phase-transfer procedure for the prepn. of benzyl ethers)

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L58 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1996:338791 HCAPLUS

DOCUMENT NUMBER: 125:58638

TITLE: Diastereoselective addition of **alkynylstannanes** to alpha stannyl substituted mixed acetals: synthesis of precursors for allenyl carbinols

AUTHOR(S): Linderman, Russell J.; Chen, Sanyou

CORPORATE SOURCE: Dep. Chemistry, North Carolina State Univ., Raleigh, NC, 27695-8204, USA

SOURCE: Tetrahedron Letters (1996), 37(22), 3819-3822

CODEN: TELEAY; ISSN: 0040-4039

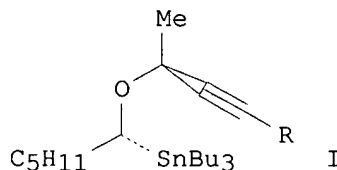
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:58638

GI



AB The regio- and stereoselective addn. of **alkynylstannanes** to stannyl substituted mixed acetals results in propargylic ether derivs. in excellent yields. Thus, Me<sub>3</sub>SiOTf mediated reaction of Bu<sub>3</sub>SnCH(C<sub>5</sub>H<sub>11</sub>)OCHMe with Bu<sub>3</sub>SnC.tplbond.CR (R = H, Me<sub>3</sub>Si, Ph, Bu, etc.) in CH<sub>2</sub>Cl<sub>2</sub> gave propargylic ether derivs. I regio- and stereoselectively.

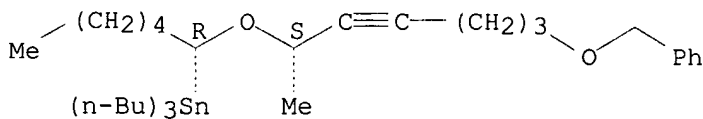
IT 178326-20-0P 178326-25-5P

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
(prepn. of)

RN 178326-20-0 HCAPLUS

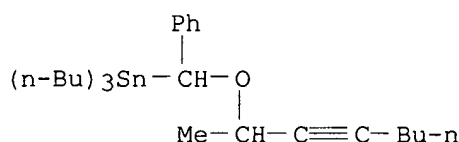
CN Stannane, tributyl[1-[1-[5-(phenylmethoxy)-1-pentynyl]ethoxy]hexyl]-, (R\*,S\*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 178326-25-5 HCAPLUS

CN Stannane, tributyl[[1-methyl-2-heptynyl]oxy]phenylmethyl]- (9CI) (CA INDEX NAME)



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- L58 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2002 ACS  
 CC 29-8 (Organometallic and Organometalloidal Compounds)  
 Section cross-reference(s): 23  
 ST diastereoselective reaction **alkynyl** stannane stannyl acetal;  
 precursor allenyl carbinol prepn; propargylic ether prepn stereochem  
 IT **Ethers, preparation**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (propargylic; synthesis of precursors for allenyl carbinols via  
 diastereoselective addn. of **alkynylstannanes** to alpha stannyl  
 substituted mixed acetals)  
 IT Regiochemistry  
 Stereochemistry  
 (synthesis of precursors for allenyl carbinols via diastereoselective  
 addn. of **alkynylstannanes** to alpha stannyl substituted mixed  
 acetals)  
 IT Acetals  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis of precursors for allenyl carbinols via diastereoselective  
 addn. of **alkynylstannanes** to alpha stannyl substituted mixed  
 acetals)  
 IT Alcohols, preparation  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (synthesis of precursors for allenyl carbinols via diastereoselective  
 addn. of **alkynylstannanes** to alpha stannyl substituted mixed  
 acetals)  
 IT 143952-57-2 178326-15-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (attempted reaction with stannyl substituted mixed acetal)  
 IT 22174-60-3P 178326-16-4P 178326-17-5P 178326-18-6P 178326-19-7P  
**178326-20-0P** 178326-21-1P 178326-22-2P 178326-23-3P  
 178326-24-4P **178326-25-5P** 178326-26-6P 178326-27-7P  
 178326-28-8P  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (prepn. of)  
 IT 994-89-8 3757-88-8 35864-20-1 81353-38-0 113248-97-8 123027-88-3  
 143304-34-1 172875-27-3 172875-35-3 178326-12-0 178326-13-1  
 178326-14-2  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (synthesis of precursors for allenyl carbinols via diastereoselective  
 addn. of **alkynylstannanes** to alpha stannyl substituted mixed  
 acetals)

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L58 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1993:254095 HCAPLUS

DOCUMENT NUMBER: 118:254095

TITLE: Direct formation of reactive  
**alkynyltrichlorotins** from 1-alkynes,  
 stannic chloride, and tributylamine. A mild  
**alkynylation** reagent of aldehydes, acetals,  
 and enones

AUTHOR(S): Yamaguchi, Masahiko; Hayashi, Akio; Hirama, Masahiro

CORPORATE SOURCE: Fac. Sci., Tohoku Univ., Sendai, 980, Japan

SOURCE: Chem. Lett. (1992), (12), 2479-82

CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 118:254095

AB A reagent system of 1-alkyne, SnCl<sub>4</sub>, and Bu<sub>3</sub>N

**alkynylates** aldehydes, acetals, and enones under mild reaction  
 conditions giving **acetylenic** alcs., **acetylenic** ethers,  
 and **acetylenic** ketones, resp., in high yields.

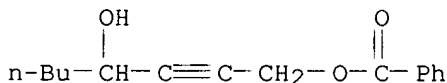
**Alkynyltrichlorotins** are shown to be the reactive species for  
 these reactions. Thus, reaction of PhC.tplbond.CH with Bu<sub>3</sub>N and SnCl<sub>4</sub> in  
 CH<sub>2</sub>Cl<sub>2</sub> followed by treatment with cyclohexanecarboxaldehyde in CH<sub>2</sub>Cl<sub>2</sub> gave  
 88% PhC.tplbond.CCHOHR (R = cyclohexyl) after quenching with H<sub>2</sub>O.

IT 146491-88-5P 146491-93-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of)

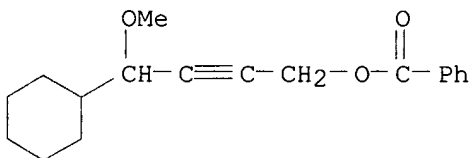
RN 146491-88-5 HCAPLUS

CN 2-Octyne-1,4-diol, 1-benzoate (9CI) (CA INDEX NAME)



RN 146491-93-2 HCAPLUS

CN 2-Butyn-1-ol, 4-cyclohexyl-4-methoxy-, benzoate (9CI) (CA INDEX NAME)



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L58 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2002 ACS

CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 29

ST **alkynylation** reagent aldehyde acetal enone;  
**alkynyltrichlorostannane**; **alkyne** reaction stannic  
 chloride tributylamine; **acetylenic** alc ether ketone

- IT Acetals  
Aldehydes, reactions  
RL: RCT (Reactant)  
(alkynylation of, reagent for)
- IT Alkynylation  
(of aldehydes, acetals, and enones, reagent for)
- IT Ethers, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(acetylenic, prepn. of, by reaction of acetals with  
alkynes in presence of tin tetrachloride and tributylamine)
- IT Alcohols, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(acetylenic, prepn. of, by reaction of aldehydes with  
alkynes in presence of tin tetrachloride and tributylamine)
- IT Ketones, preparation  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(acetylenic, prepn. of, by reaction of enones with  
alkynes in presence of tin tetrachloride and tributylamine)
- IT Ketones, reactions  
RL: RCT (Reactant)  
(unsatd., alkynylation of, reagent for)
- IT 136053-34-4  
RL: RCT (Reactant)  
(alkynylation by, of acetals in presence of tin tetrachloride  
and tributylamine)
- IT 536-74-3, Phenylacetylene 930-51-8 937-31-5, 4-  
Nitrophenylacetylene 6750-04-5 16520-62-0  
RL: RCT (Reactant)  
(alkynylation by, of aldehydes, acetals, and enones in  
presence of tin tetrachloride and tributylamine)
- IT 102-82-9, Tributylamine  
RL: RCT (Reactant)  
(alkynylation of aldehydes, acetals, and enones in presence  
of tin tetrachloride, alkynes, and)
- IT 7646-78-8, Tin tetrachloride, reactions  
RL: RCT (Reactant)  
(alkynylation of aldehydes, acetals, and enones in presence  
of tributylamine, alkynes, and)
- IT 94-41-7 104-53-0, Benzenepropanal 110-62-3, Pentanal 124-13-0,  
Octanal 149-73-5 538-58-9 630-19-3 2043-61-0,  
Cyclohexanecarboxaldehyde 18231-08-8 28833-54-7 30076-98-3  
RL: RCT (Reactant)  
(alkynylation of, reagent for)
- IT 21890-32-4P 146491-81-8P 146491-97-6P 146491-98-7P  
RL: FORM (Formation, nonpreparative); PREP (Preparation)  
(formation of, as intermediate in reaction of phenylacetylene  
with tin tetrachloride in presence of tributylamine)
- IT 34877-80-0P 58335-32-3P 80832-34-4P 114262-84-9P 130708-23-5P  
134260-67-6P 134260-71-2P 134260-73-4P 134260-74-5P 134260-75-6P  
146491-85-2P 146491-86-3P 146491-87-4P 146491-88-5P  
146491-89-6P 146491-90-9P 146491-91-0P 146491-92-1P  
146491-93-2P 146491-94-3P 146491-95-4P 146491-96-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

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L58 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1975:514545 HCAPLUS

DOCUMENT NUMBER: 83:114545

TITLE: Synthesis and transformations of p-methylbenzylpropargyl ether

AUTHOR(S): Shikhiyev, I. A.; Dzhaferov, D. S.; Karaev, S.F.

CORPORATE SOURCE: Azerb. Inst. Nefti Khim. im. Azizbekova, Baku, USSR

SOURCE: Zh. Obshch. Khim. (1975), 45(6), 1340-3

CODEN: ZOKHA4

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB P-MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>OCH<sub>2</sub>C.tplbond.CH (I) was prepd. by the reaction of ClCH<sub>2</sub>OCH<sub>2</sub>C.tplbond.CH with p-MeC<sub>6</sub>H<sub>4</sub>MgBr. Treatment of I with EtMgBr gave p-MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>OCH<sub>2</sub>C.tplbond.CMgBr which with R<sub>3</sub>SiCl gave p-MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>OCH<sub>2</sub>C.tplbond.CSiR<sub>3</sub> (R = Me, Et). I with HCHO and R<sub>1</sub>HN in presence of CuCl gave p-MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>OCH<sub>2</sub>C.tplbond.CCH<sub>2</sub>NR<sub>1</sub> (R<sub>1</sub> = Et, Me<sub>2</sub>CH; NR<sub>1</sub> = piperidino, morpholino). Reaction of I with R<sub>2</sub>R<sub>3</sub>SiH gave p-MeC<sub>6</sub>H<sub>4</sub>CH<sub>2</sub>OCH<sub>2</sub>CH:CHSiR<sub>2</sub>R<sub>3</sub> (R<sub>2</sub> = R<sub>3</sub> = Et; R<sub>2</sub> = Me<sub>2</sub>CH, R<sub>3</sub> = Me; R<sub>2</sub> = R<sub>3</sub> = EtO).

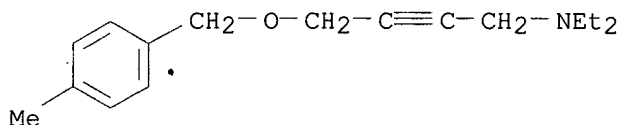
IT 56818-49-6P 56818-50-9P 56818-51-0P

56869-38-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

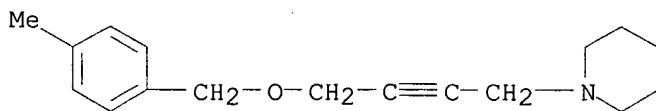
RN 56818-49-6 HCAPLUS

CN 2-Butyn-1-amine, N,N-diethyl-4-[(4-methylphenyl)methoxy]- (9CI) (CA INDEX NAME)



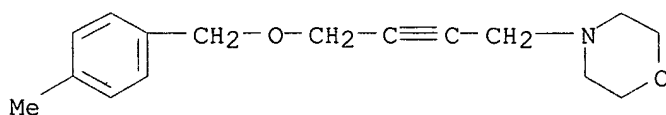
RN 56818-50-9 HCAPLUS

CN Piperidine, 1-[4-[(4-methylphenyl)methoxy]-2-butynyl]- (9CI) (CA INDEX NAME)



RN 56818-51-0 HCAPLUS

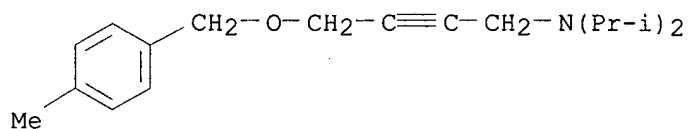
CN Morpholine, 4-[4-[(4-methylphenyl)methoxy]-2-butynyl]- (9CI) (CA INDEX NAME)



REYES 10/088,455

RN 56869-38-6 HCAPLUS

CN 2-Butyn-1-amine, N,N-bis(1-methylethyl)-4-[(4-methylphenyl)methoxy]- (9CI)  
(CA INDEX NAME)





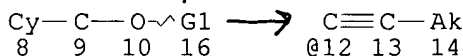
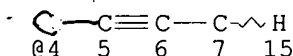
# Reg/HCA PLUS SEARCH

REYES 10/088,455

parent search } Based on Applicant's version of the rxn

=> d que 173

L1



this is a search for prep of the species

VAR G1=4/12

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 4

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

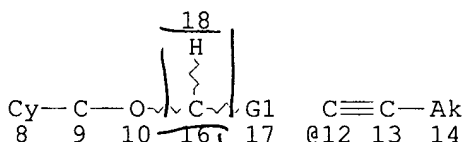
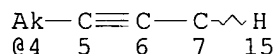
STEREO ATTRIBUTES: NONE

L2 ( 2206)SEA FILE=REGISTRY SSS FUL L1

L3 ( 2197)SEA FILE=REGISTRY ABB=ON PLU=ON L2/COM

L4 STR

subset search for product



product gets this new carbon here

VAR G1=4/12

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 4

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L5 2046 SEA FILE=REGISTRY SUB=L3 SSS FUL L4

L33 647 SEA FILE=HCAPLUS ABB=ON PLU=ON L5/PREP

L50 3884 SEA FILE=HCAPLUS ABB=ON PLU=ON ETHERS, PREPARATION/CT

L52 17 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 AND L33

L58 6 SEA FILE=HCAPLUS ABB=ON PLU=ON L52 AND (?ALKYN? OR ?ACETYLEN?)

L67 1 SEA FILE=REGISTRY ABB=ON PLU=ON

L69 6 SEA FILE=HCAPLUS ABB=ON PLU=ON

L73 4 SEA FILE=HCAPLUS ABB=ON PLU=ON

185676-84-0 rxn for daim specie  
only six preps for it

only 4 preps after subtracting out other

=&gt; d ibib abs hitstr 173 1

L73 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 2000:475622 HCAPLUS  
 DOCUMENT NUMBER: 133:89320  
 TITLE: Method for preparing a benzyl-type ether  
 INVENTOR(S): Jacquot, Roland; Spagnol, Michel  
 PATENT ASSIGNEE(S): Rhodia Chimie, Fr.  
 SOURCE: PCT Int. Appl., 62 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000040535	A1	20000713	WO 2000-FR24	20000107
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
FR 2788269	A1	20000713	FR 1999-171	19990108
FR 2788269	B1	20010209		
EP 1140758	A1	20011010	EP 2000-900536	20000107
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
PRIORITY APPLN. INFO.:			FR 1999-171	A 19990108
			WO 2000-FR24	W 20000107

OTHER SOURCE(S): CASREACT 133:89320; MARPAT 133:89320

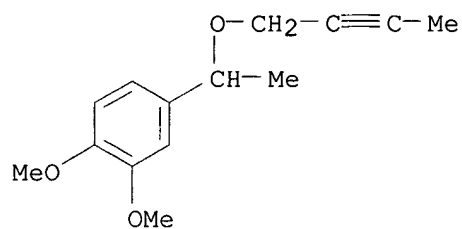
AB Benzyl ethers of arom. compds. are prepd. by first acylating the arom. compd. with an acylating agent in the presence of a zeolite or a Friedel-Crafts catalyst to form a ketone; reducing the carbonyl group into carbinol to form a benzylic alc.; etherifying the hydroxyl group by reaction with another alc. in the presence of a zeolite catalyst. Thus, veratrol was acetylated in presence of an H-Y zeolite of FeCl<sub>3</sub>; the resulting acetylveratrol was reduced over Raney Ni to give 1-(3,4-dimethoxyphenyl)ethanol which was treated with 2-butyne-1-ol in presence of a H-Y zeolite to give 96% 1-[1-(3,4-dimethoxyphenyl)ethoxy]-2-butyne.

IT 185676-84-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (prepn. of benzyl ethers from arom. hydrocarbons using zeolite catalysts)

RN 185676-84-0 HCAPLUS

CN Benzene, 4-[1-(2-butyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L73 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:64755 HCAPLUS

DOCUMENT NUMBER: 130:129961

TITLE: Method for etherifying a benzyl alcohol for  
manufacture of perfumes

INVENTOR(S): Jacquot, Roland; Spagnol, Michel

PATENT ASSIGNEE(S): Rhodia Chimie, Fr.

SOURCE: PCT Int. Appl., 38 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9902475	A1	19990121	WO 1998-FR1472	19980708
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
FR 2765870	A1	19990115	FR 1997-8733	19970709
FR 2765870	B1	19990903		
AU 9885457	A1	19990208	AU 1998-85457	19980708
EP 994838	A1	20000426	EP 1998-936479	19980708
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI			
NO 2000000065	A	20000308	NO 2000-65	20000106
US 6362378	B1	20020326	US 2000-462432	20000314
PRIORITY APPLN. INFO.:			FR 1997-8733	A 19970709
			WO 1998-FR1472	W 19980708

OTHER SOURCE(S): MARPAT 130:129961

AB A method for etherifying a benzyl alc., the resulting products and their applications in particular in perfume manuf. is disclosed. The etherification method consists in reacting a benzyl alc. with another alc. in the presence of a catalyst, characterized in that the etherification reaction is carried out in the presence of an effective amt. of a zeolite. Vanillyl alc. 5, ethanol 25, and a catalyst (40% alumina and 60% .beta.-zeolite) 2 g were heated for 2 h at 80.degree. then filtered and Et 4-hydroxy-3-methoxybenzyl ether (I) was sepd. by distn. I had an odor of burnt almond.

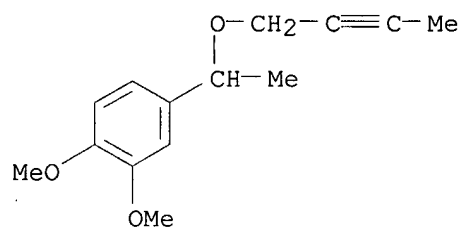
IT 185676-84-0P

RL: BUU (Biological use, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(method for etherifying benzyl alc. for manuf. of perfumes)

RN 185676-84-0 HCAPLUS

CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

12

THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d ibib abs hitstr 173 3

L73 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1998:352797 HCAPLUS

DOCUMENT NUMBER: 129:40971

TITLE: Process for the preparation of benzyl ethers

INVENTOR(S): Arvai, Geza; Bertok, Bela; Kuruczne, Ribai Zsuzsanna; Pap, Laszlo; Szekely, Istvan

PATENT ASSIGNEE(S): Chinoin Gyogyszer es Vegyeszeti Termekek Gyara Rt., Hung.; Bertok, Bela; Kuruczne Ribai, Zsuzsanna; Pap, Laszlo; Szekely, Istvan

SOURCE: PCT Int. Appl., 30 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

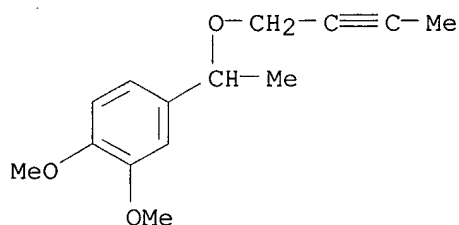
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9822416	A1	19980528	WO 1997-HU73	19971112
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9850643	A1	19980610	AU 1998-50643	19971112
AU 736832	B2	20010802		
EP 939749	A1	19990908	EP 1997-913348	19971112
EP 939749	B1	20010718		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
CN 1237954	A	19991208	CN 1997-199819	19971112
BR 9713038	A	20000411	BR 1997-13038	19971112
JP 2001505200	T2	20010417	JP 1998-523373	19971112
AT 203231	E	20010815	AT 1997-913348	19971112
ES 2161452	T3	20011201	ES 1997-913348	19971112
ZA 9710322	A	19980610	ZA 1997-10322	19971114
NO 9902375	A	19990714	NO 1999-2375	19990518
KR 2000053346	A	20000825	KR 1999-704370	19990518
US 6320085	B1	20011120	US 1999-297824	19990713
PRIORITY APPLN. INFO.:			HU 1996-3179	A 19961118
			WO 1997-HU73	W 19971112

OTHER SOURCE(S): CASREACT 129:40971; MARPAT 129:40971

AB Mixed ethers ArCR1R2OR3 [Ar = (un)substituted alicyclic, arom. or .gtoreq.1 heteroatom-contg. heterocyclic moiety; R1, R2 = H, C1-4 (halo)alkyl, C2-4 alkenyl, (un)substituted Ph, C3-6 cycloalkyl; R3 = (un)substituted C1-6 alkyl, C3-6 alkenyl, C3-6 alkynyl, etc.], chem. intermediates or arthropodicide synergists (no data), were prep'd. by etherification of alcs. R3OH (R3 as defined) with compds. ArCR1R2X (X = OH, halo, sulfo ester; R1, R2 as defined) in salt solns., in the presence of strong (mineral or org.) acids, Lewis acids, metal oxides or carbonates. For example, a mixt. of aq. CaCl2/HCl soln. (prepn. given) and 2-butyne-1-ol was added to a vigorously stirred mixt. of .alpha.-methylveratryl alc. and 2-butyne-1-ol at a fast rate and the whole was stirred for 6 h to give 94% 1-[1-(but-2-ynoxy)ethyl]-3,4-

dimethoxybenzene as colorless oil (nD20 1.5280).  
 IT **185676-84-0P**  
 RL: SPN (Synthetic preparation); **PREP (Preparation)**  
 (process for prepn. of benzyl ethers by etherification of alcs. in  
 presence of acids, Lewis acids, metal oxides and aq. salt solns.)  
 RN 185676-84-0 HCAPLUS  
 CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



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L73 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:440220 HCAPLUS

DOCUMENT NUMBER: 127:81238

TITLE: Preparation of organic pesticides with insecticide and acaricide activity

INVENTOR(S): Arvai, Geza; Bakonyvari, Ildiko; Bertok, Bela; Csiz, Laszlo; Czudor, Iren; Kuruczne, R. Zsuzsa; Pap, Laszlo; Szekely, Istvan

PATENT ASSIGNEE(S): Chinoiin Gyogyszer Es Vegyeszeti Termekkek Gyara Rt.To U. 1-5h-1045 Budapest, Hung.; Bakonyvari, Ildiko; Bertok, Bela; Csiz, Laszlo; Czudor, Iren; Kuruczne, R. Zsuzsa; Pap, Laszlo; Szekely, Istvan

SOURCE: PCT Int. Appl., 60 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9719040	A2	19970529	WO 1996-HU69	19961119
WO 9719040	A3	19970703		
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
HU 76129	A2	19970630	HU 1995-3318	19951121
CA 2238186	AA	19970529	CA 1996-2238186	19961119
AU 9677051	A1	19970611	AU 1996-77051	19961119
AU 710995	B2	19991007		
EP 862545	A2	19980909	EP 1996-940053	19961119
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2000500762	T2	20000125	JP 1997-519528	19961119
BR 9611643	A	20000308	BR 1996-11643	19961119
ZA 9609733	A	19970617	ZA 1996-9733	19961120
TW 382623	B	20000221	TW 1996-85114244	19961120
NO 9802234	A	19980709	NO 1998-2234	19980515
US 6277867	B1	20010821	US 1998-68933	19980831

PRIORITY APPLN. INFO.:

HU 1995-3318	A	19951121
WO 1996-HU69	W	19961119

AB The title compds R9C:N-group (sic) [I; R9 = H, alkyl, Ph, (un)substituted Ph], useful as insecticides and acaricides, are prepd. and I-contg. formulations presented. Thus, .alpha.-methylveratryl alc. was condensed with 1-bromo-2-butyne in the presence of NaH, producing pesticidal 1-[(2-butynyloxy)ethyl]-3,4-dimethoxybenzene in 46.9% yield.

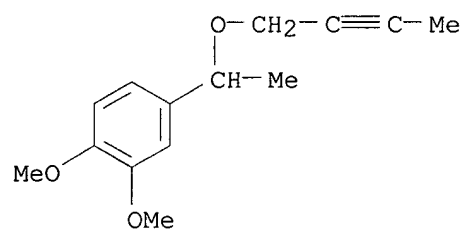
IT 185676-84-0P

RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(prepn. of org. pesticides with insecticide and acaricide activity)

RN 185676-84-0 HCAPLUS

CN Benzene, 4-[1-(2-butynyloxy)ethyl]-1,2-dimethoxy- (9CI) (CA INDEX NAME)



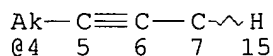


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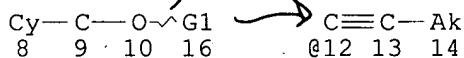
L1

STR

*parent search*



*or*



VAR G1=4/12

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 4

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

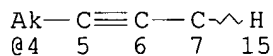
STEREO ATTRIBUTES: NONE

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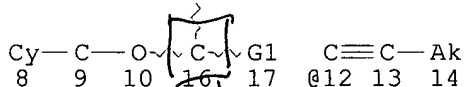
L3 ( 2197)SEA FILE=REGISTRY ABB=ON PLU=ON L2/COM

L4 STR

*product subset search*



18  
H



*new carbon*

VAR G1=4/12

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 4

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

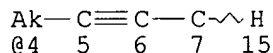
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STEREO ATTRIBUTES: NONE

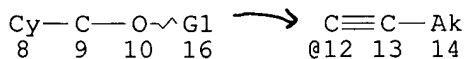
L5 2046 SEA FILE=REGISTRY SUB=L3 SSS FUL L4

L6 STR

*reactant subset search*



*or*



VAR G1=4/12

## NODE ATTRIBUTES:

CONNECT IS E2 RC AT 4  
 DEFAULT MLEVEL IS ATOM  
 DEFAULT ECLEVEL IS LIMITED

## GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED  
 NUMBER OF NODES IS 12

## STEREO ATTRIBUTES: NONE

L7 ( 2206) SEA FILE=REGISTRY SSS FUL L6  
 L8 2197 SEA FILE=REGISTRY ABB=ON PLU=ON L7/COM  
 L10 18 SEA FILE=REGISTRY ABB=ON PLU=ON C2H6O4S/MF  
 L11 10 SEA FILE=REGISTRY ABB=ON PLU=ON L10 AND ("SULFATE" OR  
 "SULFURIC")  
 L12 1 SEA FILE=REGISTRY ABB=ON PLU=ON IODOMETHANE/CN  
 L13 1 SEA FILE=REGISTRY ABB=ON PLU=ON CHLOROMETHANE/CN  
 L14 1 SEA FILE=REGISTRY ABB=ON PLU=ON BROMOETHANE/CN  
 L15 1 SEA FILE=REGISTRY ABB=ON PLU=ON CHLOROMETHANE/CN  
 L16 1 SEA FILE=REGISTRY ABB=ON PLU=ON BROMOMETHANE/CN  
 L17 3 SEA FILE=REGISTRY ABB=ON PLU=ON LDA/CN  
 L18 1 SEA FILE=REGISTRY ABB=ON PLU=ON L17 AND LI/ELS  
 L19 1 SEA FILE=REGISTRY ABB=ON PLU=ON 999-97-3  
 L20 3 SEA FILE=REGISTRY ABB=ON PLU=ON "C6H18 N SI2"/MF  
 L33 647 SEA FILE=HCAPLUS ABB=ON PLU=ON L5/PREP  
 L34 469 SEA FILE=HCAPLUS ABB=ON PLU=ON L8/RCT  
 L35 319 SEA FILE=HCAPLUS ABB=ON PLU=ON L33 AND L34  
 L36 37739 SEA FILE=HCAPLUS ABB=ON PLU=ON (L11 OR L12 OR L13 OR L14 OR  
 L15 OR L16 OR L17 OR L18 OR L19 OR L20)  
 L37 20942 SEA FILE=HCAPLUS ABB=ON PLU=ON L36(L) RCT/RL  
 L51 63545 SEA FILE=HCAPLUS ABB=ON PLU=ON ALKYNES+NT/CT  
 L60 109 SEA FILE=HCAPLUS ABB=ON PLU=ON L35 AND L51  
 L61 43 SEA FILE=HCAPLUS ABB=ON PLU=ON L60 AND ?ETHER?  
 L62 3 SEA FILE=HCAPLUS ABB=ON PLU=ON L61 AND L37  
 L64 5 SEA FILE=HCAPLUS ABB=ON PLU=ON L61 AND (ALKYLAT? OR METHYLAT?  
 OR ETHYLAT?)  
 L65 8 SEA FILE=HCAPLUS ABB=ON PLU=ON L62 OR L64

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L65 ANSWER 1 OF 8 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2001:527038 HCAPLUS

DOCUMENT NUMBER: 135:288959

TITLE: Synthesis of enantiopure 1-alkoxyallenes and their 3-alkylated derivatives

AUTHOR(S): Hausherr, Arndt; Orschel, Beate; Scherer, Stefan; Reissig, Hans-Ulrich

CORPORATE SOURCE: Institut fur Chemie - Organische Chemie, Freie Universitat Berlin, Berlin, 14195, Germany

SOURCE: Synthesis (2001), (9), 1377-1385

CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A series of enantiopure 1-alkoxyallenes  $\text{ROCH:C:CH}_2$  (R = protected carbohydrate or (-)-beta-fenchol) was prepd. starting from propargyl bromide and the corresponding optically active alcs. via propargyl ethers  $\text{ROCH}_2\text{C.tplbond.CH}$  as intermediates. In addn., disubstituted enantiopure allene derivs.  $\text{ROCH:C:CHR}_1$  (I; R = protected carbohydrate;  $\text{R}_1 = (\text{CH}_2)_8\text{CH}_3$ ) were synthesized by isomerization of the corresponding alkynes, with a ratio of isomers ranging from 1:1 to 3:1. One allene I was also prepd. via an alternative route with  $\text{ROC(TMS)C:C:CH}_2$  (R = di-O-isopropylidene-.alpha.-D-glucofuranose) as crucial intermediate.

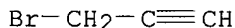
IT 106-96-7, Propargyl bromide

RL: RCT (Reactant); RACT (Reactant or reagent)

(prepn. of alkoxyallenes and their alkylated derivs. using chiral alcs. as chiral auxiliaries)

RN 106-96-7 HCAPLUS

CN 1-Propyne, 3-bromo- (9CI) (CA INDEX NAME)



IT 364733-17-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

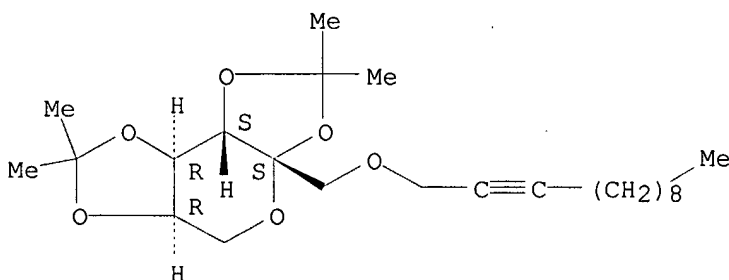
(Preparation); RACT (Reactant or reagent)

(prepn. of alkoxyallenes and their alkylated derivs. using chiral alcs. as chiral auxiliaries)

RN 364733-17-5 HCAPLUS

CN .beta.-D-Fructopyranose, 1-O-2-dodecynyl-2,3:4,5-bis-O-(1-methylethylidene)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REYES 10/088,455

REFERENCE COUNT:

31

THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d ibib abs hitstr 2

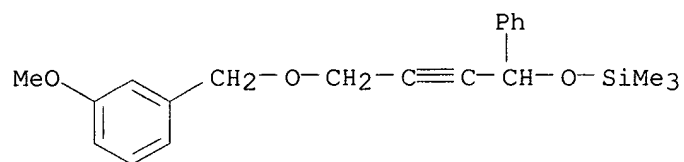
L65 ANSWER 2 OF 8 HCAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 2001:375616 HCAPLUS  
 DOCUMENT NUMBER: 135:122019  
 TITLE: Novel Carbon-Carbon Bond-Forming Reactions Using Carbocations Produced from Substituted Propargyl Silyl **Ethers** by the Action of TMSOTf  
 AUTHOR(S): Ishikawa, Teruhiko; Okano, Masamitsu; Aikawa, Toshiaki; Saito, Seiki  
 CORPORATE SOURCE: Department of Bioscience and Biotechnology Faculty of Engineering, Okayama University, Tsushima Okayama, 700-8530, Japan  
 SOURCE: Journal of Organic Chemistry (2001), 66(13), 4635-4642  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 135:122019  
 AB Highly useful carbon-carbon bond forming reactions using stable allenyl, propargyl, or allyl-propargyl hybrid cations have been developed. These carbocations could be generated from silyl 1-( $\pi$ -donor)-substituted propargyl **ethers** by the action of trimethylsilyl trifluoromethanesulfonate in dichloromethane at  $-78^{\circ}\text{C}$  to room temp. and could be attacked nucleophilically by electron rich arenes, allylsilanes, or enol silyl **ethers**, giving rise to allenes, alkynes, and their derivs. A novel method for regio- and stereoselective synthesis of conjugated enynes utilizing allyl-propargyl hybrid cations has also been established.  
 IT 536-74-3, Phenylacetylene 1066-54-2, Trimethylsilylacetylene  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (carbon-carbon bond-forming reactions using carbocations produced from substituted propargyl silyl **ethers** by the action of TMSOTf)  
 RN 536-74-3 HCAPLUS  
 CN Benzene, ethynyl- (8CI, 9CI) (CA INDEX NAME)

Ph-C $\equiv$ CH

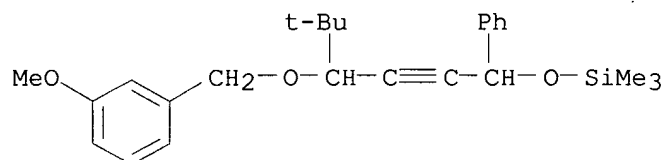
RN 1066-54-2 HCAPLUS  
 CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me<sub>3</sub>Si-C $\equiv$ CH

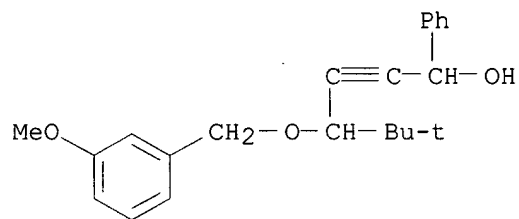
IT 350693-39-9P 350693-41-3P 350693-44-6P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (carbon-carbon bond-forming reactions using carbocations produced from substituted propargyl silyl **ethers** by the action of TMSOTf)  
 RN 350693-39-9 HCAPLUS  
 CN Silane, [[4-[(3-methoxyphenyl)methoxy]-1-phenyl-2-butylnyl]oxy]trimethyl- (9CI) (CA INDEX NAME)



RN 350693-41-3 HCAPLUS  
 CN Silane, [[4-[(3-methoxyphenyl)methoxy]-5,5-dimethyl-1-phenyl-2-hexynyl]oxy]trimethyl- (9CI) (CA INDEX NAME)



RN 350693-44-6 HCAPLUS  
 CN Benzenemethanol, .alpha.-[3-[(3-methoxyphenyl)methoxy]-4,4-dimethyl-1-pentynyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS .  
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d ibib abs hitstr 3

L65 ANSWER 3 OF 8 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1999:282451 HCAPLUS

DOCUMENT NUMBER: 131:19258

TITLE: Synthesis of viridiofungin A and its absolute structure

AUTHOR(S): Esumi, T.; Iwabuchi, Y.; Irie, H.; Hatakeyama, S.

CORPORATE SOURCE: Faculty of Pharmaceutical Sciences, Nagasaki University, Nagasaki, Japan

SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1997), 39th, 409-414

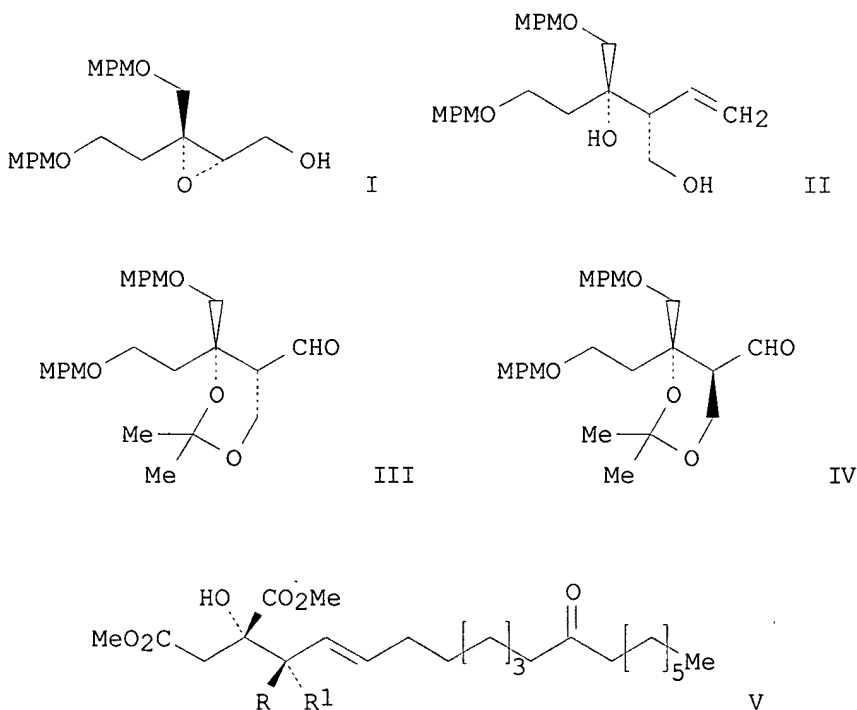
CODEN: TYKYDS

PUBLISHER: Nippon Kagakkai

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

GI



AB Viridiofungin A was isolated from a strain of *Trichoderma viride* Pers. (Fungi, Hyphomycetes) **together** with viridiofungin B and C after screening for substances that exhibit cholesterol lowering activity. These viridiofungins, a novel family of squalene synthase inhibitors, have unique structures consisting of a common citric acid moiety having C-16 long chain and an arom. amino acid residue such as tyrosine, phenylalanine, and tryptophane. However, the abs. structures of these compds. have not been detd. yet. We describe the first synthesis of viridiofungin A tri-Me ester which allowed us to det. its abs. configuration to be 3S,4S,2'S. Katsuki-Sharpless asym. epoxidn. of the trisubstituted allylic alc. [trans-MPMOCH<sub>2</sub>CH<sub>2</sub>C(CH<sub>2</sub>OMPM):CHCH<sub>2</sub>OH; MPM = p-methoxybenzyl] followed by regio- and stereoselective opening of epoxide



(I) to give the diol (II) from which two epimeric aldehydes (III and IV) were prepd. selectively. Upon attachment of the long chain portion by Wittig olefination reaction followed by functional group transformations, the aldehyde III and IV gave the alc. (V; R = H, R1 = CH2OH) and (V; R = CH2OH, R1 = H) resp. After Jones oxidn. of V (R = H, R1 = CH2OH), the resulting carboxylic acid was condensed with L- and D-tyrosine Me ester to give (3S,4S,2'S)-viridiofungin A tri-Me ester (V; R = H, R1 = L-Tyr-OMe) and (3S,4S,2'R)-viridiofungin A tri-Me ester (V; R = H, R1 = D-Tyr-OMe) (viridiofungin A deriv.). Similarly, (3S,4R,2'S)-viridiofungin A tri-Me ester (V; R = L-Tyr-OMe, R1 = H) and (3S,4R,2'R)-viridiofungin A tri-Me ester (V; R = D-Tyr-OMe, R1 = H) were also synthesized from V (R = H, R1 = CH2OH). Now we can conclude that the abs. configuration of natural viridiofungin A is 3S,4S,2'S by comparison (1H NMR and TLC) of four synthetic samples with natural viridiofungin A tri-Me ester in addn. to information that the tyrosine-configuration is L.

IT 74-88-4, reactions 927-74-2, 3-Butyn-1-ol

RL: RCT (Reactant); RACT (Reactant or reagent)

(total synthesis of viridiofungin A having cholesterol-lowering and squalene synthase inhibitory activity and its abs. structure)

RN 74-88-4 HCAPLUS

CN Methane, iodo- (8CI, 9CI) (CA INDEX NAME)

H<sub>3</sub>C-I

RN 927-74-2 HCAPLUS

CN 3-Butyn-1-ol (7CI, 8CI, 9CI) (CA INDEX NAME)

HO-CH<sub>2</sub>-CH<sub>2</sub>-C≡CH

IT 146916-76-9P, 5-(p-Methoxybenzyloxy)-2-pentyn-1-ol

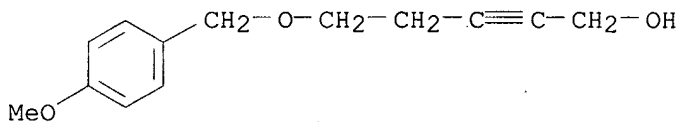
RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(total synthesis of viridiofungin A having cholesterol-lowering and squalene synthase inhibitory activity and its abs. structure)

RN 146916-76-9 HCAPLUS

CN 2-Pentyn-1-ol, 5-[(4-methoxyphenyl)methoxy]- (9CI) (CA INDEX NAME)



=&gt; d ibib abs hitstr 4

L65 ANSWER 4 OF 8 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:913284 HCAPLUS

DOCUMENT NUMBER: 123:340754

TITLE: Non-peptide peptidomimetics with affinity for G-protein-linked receptors

INVENTOR(S): Hirschmann, Ralph F.; Nicolaou, Kyriacos C.; Pietranico, Sherrie; Reisine, Terry D.; Salvino, Joseph M.; Sprengeler, Paul; Strader, Catherine D.

PATENT ASSIGNEE(S): Trustees of the University of Pennsylvania, USA

SOURCE: PCT Int. Appl., 200 pp.

CODEN: PIXXD2

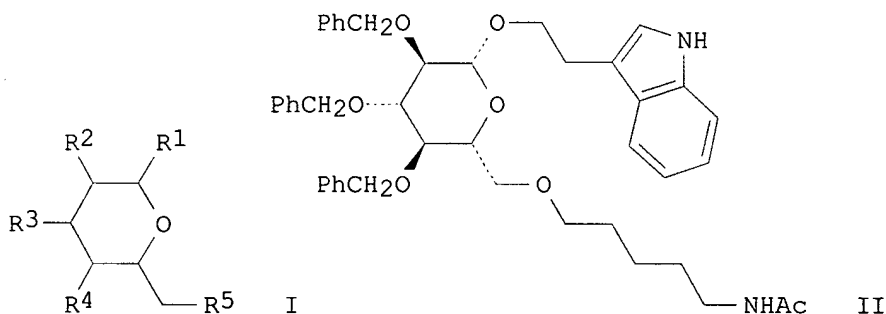
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9511686	A1	19950504	WO 1994-US12233	19941026
W: CA, JP				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
US 5552534	A	19960903	US 1993-144660	19931028
EP 728007	A1	19960828	EP 1994-932029	19941026
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
PRIORITY APPLN. INFO.:			US 1993-144660	19931028
			US 1991-748826	19910822
			WO 1994-US12233	19941026
OTHER SOURCE(S):		MARPAT 123:340754		
GI				



AB Compds. I [.gtoreq.1 of R1, R2, R3, R4 or R5 comprises a functional group chem. similar to that found in a peptide of interest] are provided. I are cross-reactive with peptides such as those which bind G-protein-linked receptors. For example, reaction of N-(phenylsulfonyl)tryptophol with 1-bromo-.alpha.-D-glucose tetraacetate [preps. given] in the presence of Ag2O gave 64% 2-(1-phenylsulfonylindol-3-yl)ethyl 2,3,4,6-tetra-O-acetyl-.beta.-D-glucopyranoside, which underwent deacetylation (88%), 6-O-silylation (85%), 2,3,4-tri-O-benzoylation (74%), desilylation (94%), conversion to the 6-O-triflate, **etherification** with AcNH(CH2)5OH using 2.2 mol equiv NaH, and deprotection of the indole N with NaOH in aq. EtOH, to give title compd. II. The IC50 of II for inhibition of substance P binding to cloned human neurokinin-1 receptor was 56 nM. Preps. of

approx. 40 compds. I and their intermediates, and binding data for selected compds. to several receptor types, are described.

IT 170219-51-9P 170219-52-0P 170219-53-1P

170219-54-2P 170219-55-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

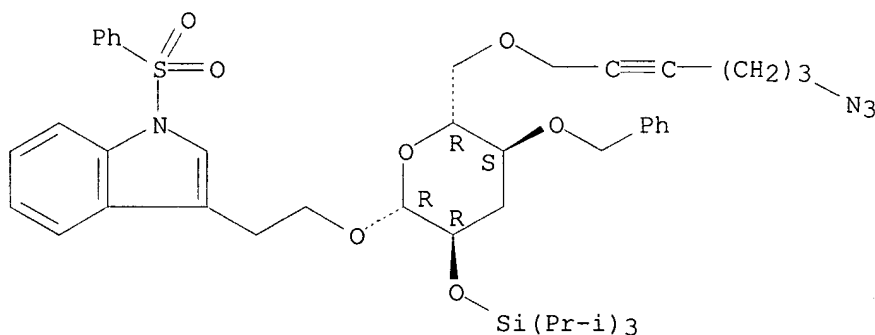
(Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of glucopyranoside-based peptidomimetics)

RN 170219-51-9 HCAPLUS

CN 1H-Indole, 3-[2-[[6-O-(6-azido-2-hexynyl)-3-deoxy-4-O-(phenylmethyl)-2-O-[tris(1-methylethyl)silyl]-.beta.-D-ribo-hexopyranosyl]oxy]ethyl]-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

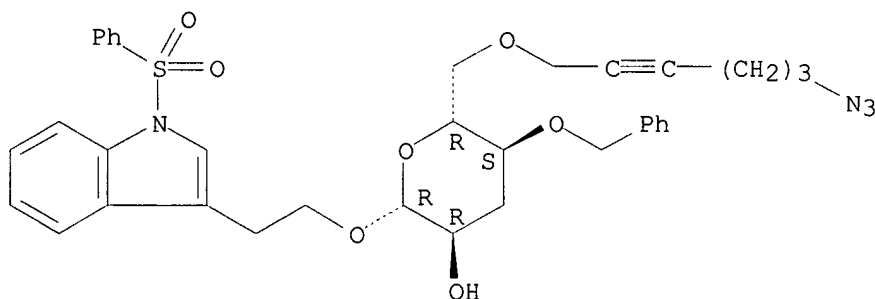
Absolute stereochemistry. Rotation (-).



RN 170219-52-0 HCAPLUS

CN 1H-Indole, 3-[2-[[6-O-(6-azido-2-hexynyl)-3-deoxy-4-O-(phenylmethyl)-.beta.-D-ribo-hexopyranosyl]oxy]ethyl]-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

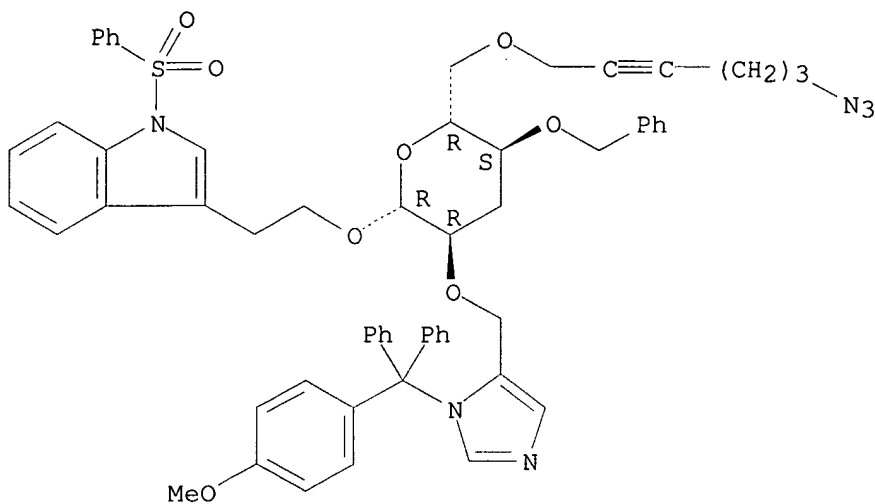
Absolute stereochemistry. Rotation (-).



RN 170219-53-1 HCAPLUS

CN 1H-Indole, 3-[2-[[6-O-(6-azido-2-hexynyl)-3-deoxy-2-O-[[1-[(4-methoxyphenyl)diphenylmethyl]-1H-imidazol-5-yl]methyl]-4-O-(phenylmethyl)-.beta.-D-ribo-hexopyranosyl]oxy]ethyl]-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

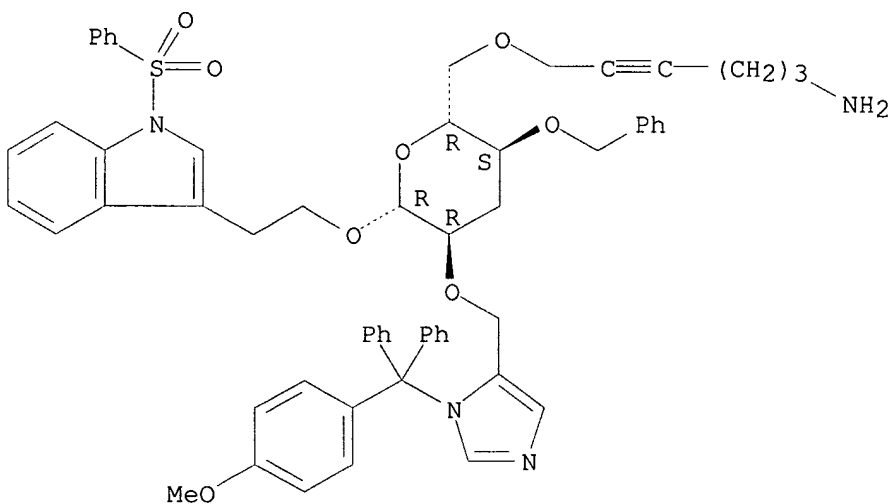
Absolute stereochemistry. Rotation (-).



RN 170219-54-2 HCAPLUS

CN 1H-Indole, 3-[2-[[6-O-(6-amino-2-hexynyl)-3-deoxy-2-O-[[1-[(4-methoxyphenyl)diphenylmethyl]-1H-imidazol-5-yl]methyl]-4-O-(phenylmethyl)-.beta.-D-ribo-hexopyranosyl]oxy]ethyl]-1-(phenylsulfonyl)- (9CI) (CA INDEX NAME)

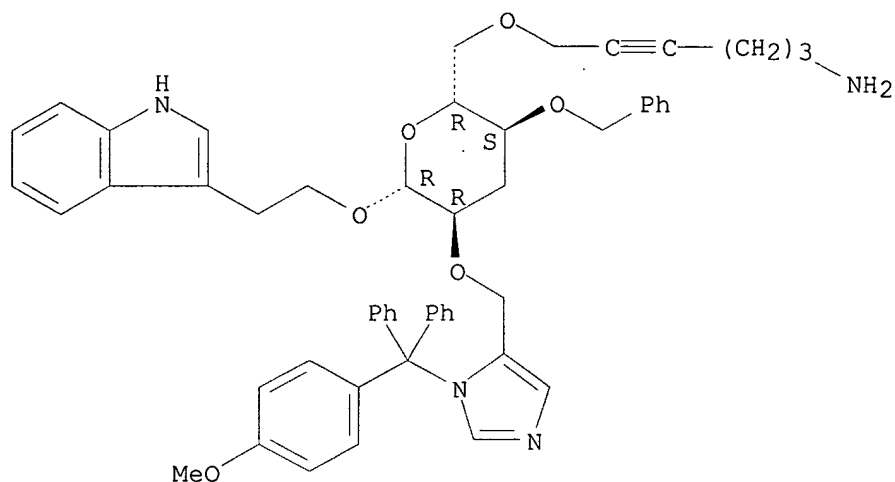
Absolute stereochemistry. Rotation (+).



RN 170219-55-3 HCAPLUS

CN .beta.-D-ribo-Hexopyranoside, 2-(1H-indol-3-yl)ethyl 6-O-(6-amino-2-hexynyl)-3-deoxy-2-O-[[1-[(4-methoxyphenyl)diphenylmethyl]-1H-imidazol-5-yl]methyl]-4-O-(phenylmethyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



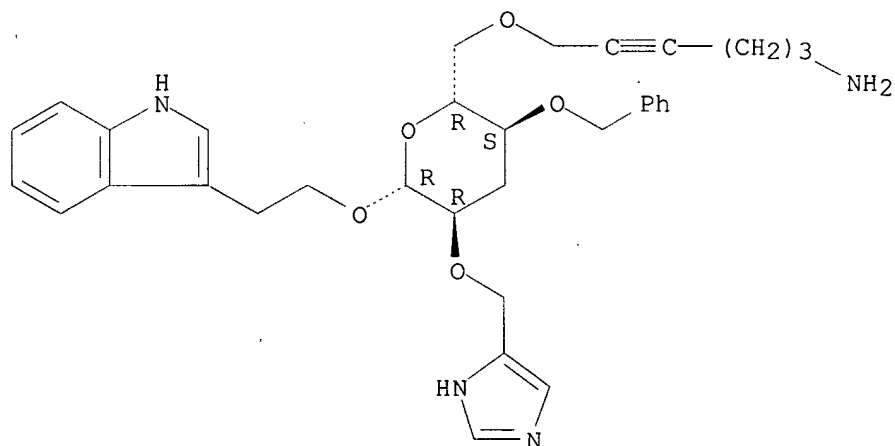
IT 170219-14-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)  
(prepn. of glucopyranoside-based peptidomimetics)

RN 170219-14-4 HCAPLUS

CN .beta.-D-ribo-Hexopyranoside, 2-(1H-indol-3-yl)ethyl 6-O-(6-amino-2-hexynyl)-3-deoxy-2-O-(1H-imidazol-4-ylmethyl)-4-O-(phenylmethyl)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 74-88-4, Methyl iodide, reactions 927-74-2, 3-Butyn-1-ol

RL: **RCT (Reactant)**; RACT (Reactant or reagent)  
(starting material; prepn. of glucopyranoside-based peptidomimetics)

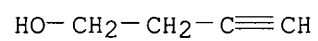
RN 74-88-4 HCAPLUS

CN Methane, iodo- (8CI, 9CI) (CA INDEX NAME)

H<sub>3</sub>C-I

REYES 10/088,455

RN 927-74-2 HCAPLUS  
CN 3-Butyn-1-ol (7CI, 8CI, 9CI) (CA INDEX NAME)



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L65 ANSWER 5 OF 8 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:700492 HCAPLUS

DOCUMENT NUMBER: 121:300492

TITLE: Pd-Catalyzed Cycloisomerization to 1,2-Dialkylidenecycloalkanes. 1

AUTHOR(S): Trost, Barry M.; Tanoury, Gerald J.; Lautens, Mark; Chan, Chuen; MacPherson, David T.

CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94035-5080, USA

SOURCE: Journal of the American Chemical Society (1994), 116(10), 4255-67

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 121:300492

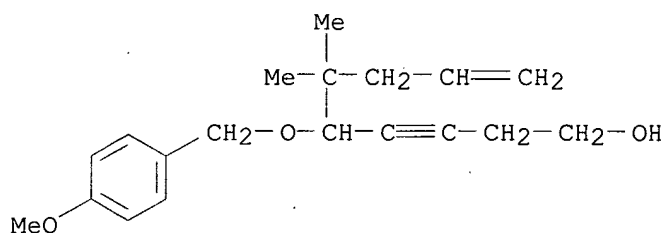
AB Enhancing synthetic efficiency requires the development of synthetic reactions that, to the extent possible, are simple addns. wherein everything else is required only in catalytic amts. The Alder ene reaction constitutes a classical reaction that meets this requirement that has much unrealized potential. A transition-metal-catalyzed version helps to increase that potential by permitting this reaction to proceed under mild conditions. A significant benefit of transition metal catalysis is the feasibility of diverting the reaction along pathways not feasible under thermal conditions. The synthesis of 1,3-dienes rather than 1,4-dienes is a very important diversion because of the utility of 1,3-dienes as reaction partners in the Diels-Alder reaction, another highly atom economical process. A catalyst derived from palladium acetate cycloisomerizes 1,6- and 1,7-enynes to dialkylidenecyclopentanes and -cyclohexanes. 1,3-Diene formation is favored over the Alder ene process by both steric and electronic effects. The reaction is highly chemoselective - tolerating a wide diversity of functionality including hydroxyl groups, ketones, esters, alkynyl and enol **ethers**, alkynyl and vinyl silanes, and enones. Many of the substrates are available by palladium-catalyzed **alkylation** reactions - highlighting the effectiveness of palladium catalyzed methodol. in org. synthesis. The atom-economical nature of these reactions combined with the Diels-Alder reaction permit butadiene and di-Me propargylmalonate to be molded into a polyhydro-as-indacene. The mechanism of this reaction may involve a tautomerization of an enyne-Pd(+2) complex to a pallada(+4)cyclopentene intermediate as a key step.

IT 159009-41-3P

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)  
(formation and **methylation** of)

RN 159009-41-3 HCAPLUS

CN 8-Nonen-3-yn-1-ol, 5-[(4-methoxyphenyl)methoxy]-6,6-dimethyl- (9CI) (CA INDEX NAME)

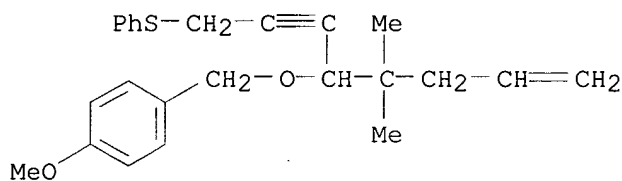


IT 159009-34-4P

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
(prepn. and attempted palladium-catalyzed cycloisomerization of)

RN 159009-34-4 HCAPLUS

CN Benzene, 1-[[[2,2-dimethyl-1-[[3-(phenylthio)-1-propynyl]-4-pentenyl]oxy]methyl]-4-methoxy- (9CI) (CA INDEX NAME)

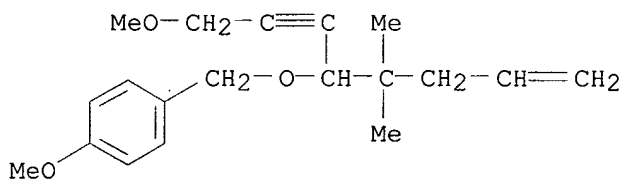


IT 159009-36-6P 159009-37-7P 159009-39-9P

RL: SPN (Synthetic preparation); **PREP (Preparation)**  
(prepn. and palladium-catalyzed cycloisomerization of)

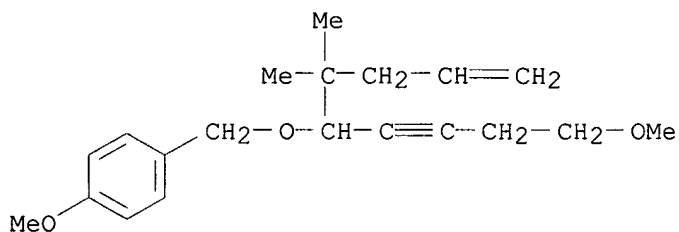
RN 159009-36-6 HCAPLUS

CN Benzene, 1-methoxy-4-[[[1-(3-methoxy-1-propynyl)-2,2-dimethyl-4-pentenyl]oxy]methyl]- (9CI) (CA INDEX NAME)



RN 159009-37-7 HCAPLUS

CN Benzene, 1-methoxy-4-[[[1-(4-methoxy-1-butynyl)-2,2-dimethyl-4-pentenyl]oxy]methyl]- (9CI) (CA INDEX NAME)

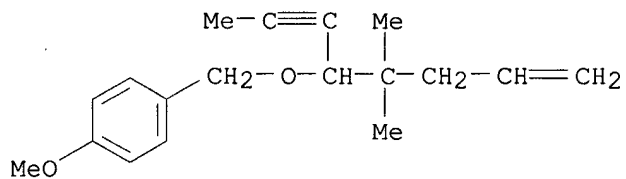


RN 159009-39-9 HCAPLUS

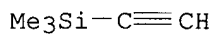
CN Benzene, 1-[[[2,2-dimethyl-1-(1-propynyl)-4-pentenyl]oxy]methyl]-4-methoxy-



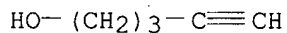
(9CI) (CA INDEX NAME)



IT 1066-54-2, (Trimethylsilyl)acetylene  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (sequential lithiation and reaction of, with dimethylpentenal)  
 RN 1066-54-2 HCAPLUS  
 CN Silane, ethynyltrimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 5390-04-5, 4-Pentyn-1-ol  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (silylation of)  
 RN 5390-04-5 HCAPLUS  
 CN 4-Pentyn-1-ol (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



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L65 ANSWER 6 OF 8 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1989:114275 HCAPLUS

DOCUMENT NUMBER: 110:114275

TITLE: Synthesis and stereochemical study of acetals of Z and E isomers of 5-alkoxy-3-hexenals and 3-alkoxy-4-hexenals

AUTHOR(S): Raifel'd, Yu. E.; Arshava, B. M.; Zil'berg, L. L.; Makin, S. M.

CORPORATE SOURCE: Mosk. Inst. Tonk. Tekhnol., Moscow, USSR

SOURCE: Zh. Org. Khim. (1988), 24(5), 939-43

CODEN: ZORKAE; ISSN: 0514-7492

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 110:114275

AB Grignard reaction of MeC.tplbond.CH with HCOCH<sub>2</sub>CH(OMe)<sub>2</sub> gave MeC.tplbond.CCH(OH)CH<sub>2</sub>CH(OMe)<sub>2</sub>, which was reduced with H over Pd/CaCO<sub>3</sub> and with LiAlH<sub>4</sub> to give Z- and E-MeCH:CHCH(OR)CH<sub>2</sub>CH(OMe)<sub>2</sub> (I; R = H), resp. Subsequent **methylation** with MeI in THF contg. NaH gave the isomeric trimethoxyhexenes in 66-78% yield. An analogous reaction sequence starting with MeCHO and HC.tplbond.CCH<sub>2</sub>CH(OMe)<sub>2</sub> gave 71-73% Z- and E-R1OCHMeCH:CHCH<sub>2</sub>CH(OMe)<sub>2</sub> (E-II; R1 = Me), while benzylation of the intermediate HOCHMeC.tplbond.CCH<sub>2</sub>CH(OMe)<sub>2</sub> followed by redn. as above gave 90% Z- and 77% E-II (R1 = PhCH<sub>2</sub>). I (R = Me) was also prepd. directly in 45% yield by treating E-MeCH:CHCH(OMe)<sub>2</sub> with CH<sub>2</sub>:CHOMe in EtOAc contg. ZnCl<sub>2</sub> and BF<sub>3</sub>.OEt<sub>2</sub>, while the Z isomer resulted from debromination of MeC.tplbond.CCH(OMe)CHXCH(OMe)<sub>2</sub> (III; X = Br) with LiAlH<sub>4</sub> in Et<sub>2</sub>O to give 79% III (X = H) followed by Lindlar redn.

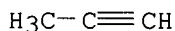
IT 74-99-7, Propyne

RL: RCT (Reactant)

(Grignard alkynylation by, of dimethoxypropionaldehyde)

RN 74-99-7 HCAPLUS

CN 1-Propyne (9CI) (CA INDEX NAME)



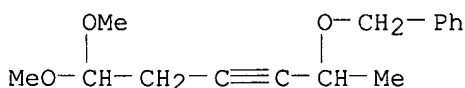
IT 119254-44-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and redn. of, stereochem. of)

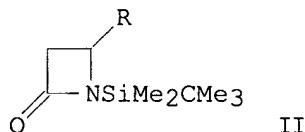
RN 119254-44-3 HCAPLUS

CN Benzene, [[5,5-dimethoxy-1-methyl-2-pentynyl]oxy]methyl]- (9CI) (CA INDEX NAME)



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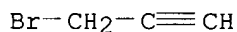
L65 ANSWER 7 OF 8 HCAPLUS COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 1987:66954 HCAPLUS  
 DOCUMENT NUMBER: 106:66954  
 TITLE: 4-Propargyl-2-azetidinone as a versatile synthon for  
 the synthesis of .beta.-lactam antibiotics:  
 hydrostannation and its reactivities  
 AUTHOR(S): Nishida, Atsushi; Shibasaki, Masakatsu; Ikegami, Shiro  
 CORPORATE SOURCE: Fac. Pharm. Sci., Teikyo Univ., Sagamiko, 199-01,  
 Japan  
 SOURCE: Chem. Pharm. Bull. (1986), 34(4), 1423-33  
 CODEN: CPBTAL; ISSN: 0009-2363  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 OTHER SOURCE(S): CASREACT 106:66954  
 GI



AB 4-Propargyl-2-azetidinone (I) was prepd. from 4-(phenylsulfonyl)-2-azetidinone by Grignard reaction with HC.tplbond.CCH2Br. I was converted to the ketones II (R = CH2COEt, CH2CH2COCHMeOAc), which are the key intermediates for the synthesis of carbapenem and carbacephem antibiotics. In this transformation polar functional groups control the regiochem. of hydrostannation of I. Other alkynes were also tributylstannylated, the resulting stannylalkenes epoxidized, and the epoxystannanes treated with HCO2H to give ketones.

IT 106-96-7, Propargylbromide  
 RL: RCT (Reactant)  
 (Grignard reaction of, with (phenylsulfonyl)azetidinone)

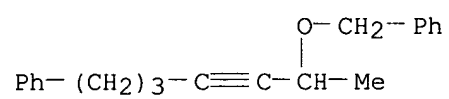
RN 106-96-7 HCAPLUS  
 CN 1-Propyne, 3-bromo- (9CI) (CA INDEX NAME)



IT 106575-42-2P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (prepn. and stannylation of)

RN 106575-42-2 HCAPLUS  
 CN Benzene, [[[1-methyl-6-phenyl-2-hexynyl)oxy]methyl]- (9CI) (CA INDEX NAME)

REYES 10/088,455



=&gt; d ibib abs hitstr 8

L65 ANSWER 8 OF 8 HCAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1976:576850 HCAPLUS

DOCUMENT NUMBER: 85:176850

TITLE: Aliphatic carbonyl compounds

INVENTOR(S): Chan, Ka-Kong; Saucy, Gabriel

PATENT ASSIGNEE(S): Hoffmann-La Roche, F., und Co., A.-G., Switz.

SOURCE: Ger. Offen., 41 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2602508	A1	19760729	DE 1976-2602508	19760123
US 4000169	A	19761228	US 1975-544153	19750127
NL 7600807	A	19760729	NL 1976-807	19760127
JP 51100012	A2	19760903	JP 1976-7194	19760127
GB 1510053	A	19780510	GB 1976-3081	19760127
FR 2399402	A1	19790302	FR 1976-2162	19760127
			US 1975-544153	19750127

PRIORITY APPLN. INFO.:

AB RCOCH<sub>2</sub>CHMeCH:CH(CH<sub>2</sub>CHMeCH<sub>2</sub>CH<sub>2</sub>)nCHR<sub>1</sub>CR<sub>2</sub>Me<sub>2</sub> I (R = H, OH, NMe<sub>2</sub>, OMe, etc.; R<sub>1</sub>R<sub>2</sub> = H, bond; n = 0, 1) were prepd. by the reaction of an unsatd. alc. with MeC(OR)<sub>2</sub>R<sub>1</sub> (R = Me, Et; R<sub>1</sub> = OR, NMe<sub>2</sub>) or a vinyl alkyl **ether**. Thus, R-cis-MeCH:CHCH(OH)CH<sub>2</sub>CHMe<sub>2</sub> was refluxed with MeC(OEt)<sub>3</sub> in EtCO<sub>2</sub>H with distn. of EtOH to give S-trans-EtO<sub>2</sub>CCH<sub>2</sub>CHMeCH:CHCH<sub>2</sub>CHMe<sub>2</sub>. I are useful for the prepn. of tocopherol derivs.

IT 74-99-7

RL: RCT (Reactant)

(Grignard reaction of, with ethyl bromide)

RN 74-99-7 HCAPLUS

CN 1-Propyne (9CI) (CA INDEX NAME)

H<sub>3</sub>C-C≡CH

IT 74-96-4

RL: RCT (Reactant)

(Grignard reaction of, with propyne)

RN 74-96-4 HCAPLUS

CN Ethane, bromo- (8CI, 9CI) (CA INDEX NAME)

Br-CH<sub>2</sub>-CH<sub>3</sub>

IT 59983-85-6P 59983-87-8P

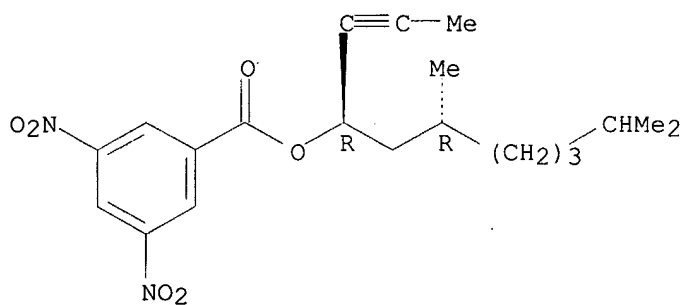
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)

(prepn. and hydrolysis of)

RN 59983-85-6 HCAPLUS

CN 2-Undecyn-4-ol, 6,10-dimethyl-, 3,5-dinitrobenzoate, [R-(R\*,R\*)]- (9CI) (CA INDEX NAME)

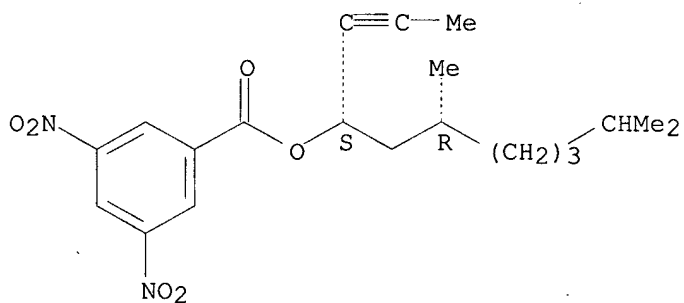
Absolute stereochemistry.



RN 59983-87-8 HCAPLUS

CN 2-Undecyn-4-ol, 6,10-dimethyl-, 3,5-dinitrobenzoate, [S-(R\*,S\*)]- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.

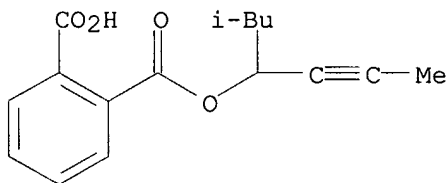


IT 59983-73-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. and resolu. of)

RN 59983-73-2 HCAPLUS

CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester  
(9CI) (CA INDEX NAME)



IT 60018-70-4P 60018-71-5P 60018-73-7P

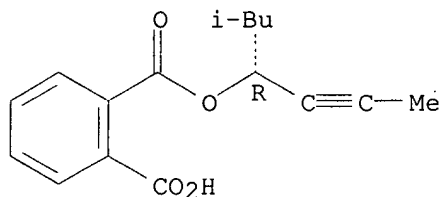
60974-93-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(prepn. of)

RN 60018-70-4 HCAPLUS

CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester,  
(R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

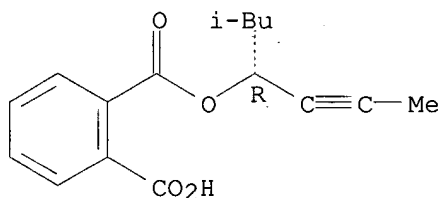


RN 60018-71-5 HCAPLUS  
 CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester,  
 (R)-, compd. with (R)-.alpha.-methylbenzenemethanamine (1:1) (9CI) (CA  
 INDEX NAME)

CM 1

CRN 60018-70-4  
 CMF C16 H18 O4

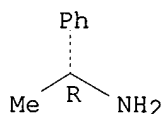
Absolute stereochemistry.



CM 2

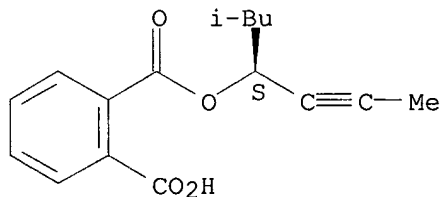
CRN 3886-69-9  
 CMF C8 H11 N

Absolute stereochemistry.



RN 60018-73-7 HCAPLUS  
 CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester,  
 (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 60974-93-8 HCAPLUS

REYES 10/088,455

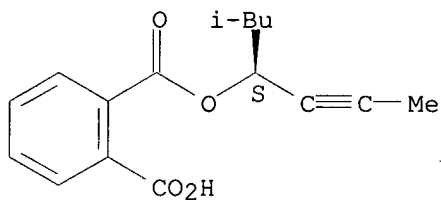
CN 1,2-Benzenedicarboxylic acid, mono[1-(2-methylpropyl)-2-butynyl] ester,  
(S)-, compd. with (S)-.alpha.-methylbenzenemethanamine (1:1) (9CI) (CA  
INDEX NAME)

CM 1

CRN 60018-73-7

CMF C16 H18 O4

Absolute stereochemistry.

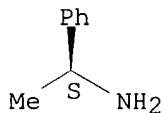


CM 2

CRN 2627-86-3

CMF C8 H11 N

Absolute stereochemistry.





CASREACT search based  
on Applicant  
version of the rxn

REYES 10/088,455

=> d que 117

L11

STR

parent rxn

RRT

PRO

Cy—C—O—G1—C≡C—C~H  
1 2 3 4 5 6 7 15

Cy—C—O~C~G1—C≡C—Ak  
8 9 10 16 11 12 13 14

REP G1=(0-10) C

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L13 112 SEA FILE=CASREACT SSS FUL L11 ( 436 REACTIONS)

L15 STR

RRT

RRT

subset rxn

Cy—C—O—G1—C≡C—C~H  
1 2 3 4 5 6 7 15

Ak~G2  
17 18

PRO

Cy—C—O~C~G1—C≡C—Ak  
8 9 10 16 11 12 13 14

O~S~O  
@19 20 21

} alkylating reagents  
added to the search

REP G1=(0-10) C

VAR G2=X/19

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 17

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L17 6 SEA FILE=CASREACT SUB=L13 SSS FUL L15 ( 19 REACTIONS)

=&gt; d ibib abs fcrdref 1

L17 ANSWER 1 OF 6 CASREACT COPYRIGHT 2002 ACS

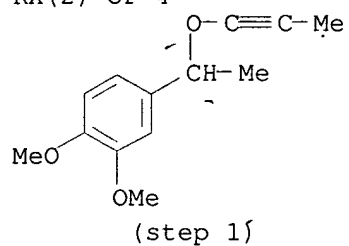
ACCESSION NUMBER: 134:266094 CASREACT  
 TITLE: Method for preparing substituted mixed alkynyl ethers  
 INVENTOR(S): Jacquot, Roland  
 PATENT ASSIGNEE(S): Rhodia Chimie, Fr.  
 SOURCE: PCT Int. Appl., 26 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: French  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001023338	A1	20010405	WO 2000-FR2704	20000929
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG FR 2798928 A1 20010330 FR 1999-12146 19990929 EP 1216220 A1 20020626 EP 2000-966235 20000929 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL PRIORITY APPLN. INFO.: FR 1999-12146 19990929 WO 2000-FR2704 20000929				

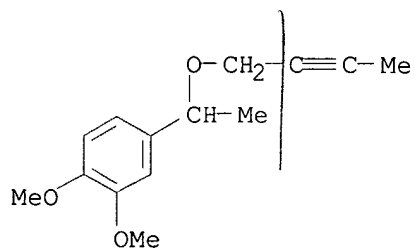
OTHER SOURCE(S): MARPAT 134:266094

AB The invention concerns a method for prepg. substituted mixed alkynyl ethers. More particularly, the invention concerns the prepn. of mixed ethers derived from a substituted benzyl alc. and an alkynyl alc. The inventive method for prepg. a substituted mixed benzyl/alkynyl ether from a mixed benzyl/alkynyl ether having a hydrogen atom on the triple bond is characterized in that it consists in reacting a mixed ether derived from a benzyl alc. and an alkynyl alc. having a hydrogen atom on the triple bond with an alkylating agent, in the presence of a neg. ion chem. ionizing reagent. E.g., methylation of [1-(prop-1-ynyloxy)ethyl]-3,4-dimethoxybenzene, prepd. by reaction of 1-[3,4-dimethoxyphenyl]ethan-1-ol with propargyl alc. in presence of HY zeolite, with Me sulfate gave [1-(but-2-ynyloxy)ethyl]-3,4-dimethoxybenzene.

RX(2) OF 4



1. NaNH<sub>2</sub>, PhMe  
 2. Me<sub>2</sub>SO<sub>4</sub>



100%

REF: PCT Int. Appl., 2001023338, 05 Apr 2001

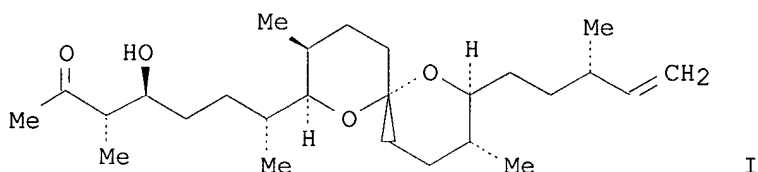
REFERENCE COUNT:

4

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d ibib abs fcrdref 2

L17 ANSWER 2 OF 6 CASREACT COPYRIGHT 2002 ACS  
 ACCESSION NUMBER: 134:237326 CASREACT  
 TITLE: Synthesis of a C1-C21 Subunit of the Protein  
 Phosphatase Inhibitor Tautomycin: A Formal Total  
 Synthesis  
 AUTHOR(S): Marshall, James A.; Yanik, Mathew M.  
 CORPORATE SOURCE: Department of Chemistry, University of Virginia,  
 Charlottesville, VA, 22904, USA  
 SOURCE: Journal of Organic Chemistry (2001), 66(4), 1373-1379  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB The synthesis of a C1-C21 subunit of tautomycin is described. The convergent route employs enantioenriched allenylstannane and zinc reagents derived from (S)-3-butyn-2-ol methanesulfonate. These reagents react with appropriate aldehyde segments to yield syn and anti adducts with high diastereoselectivity. The derived lithioalkynes are joined stepwise to a CO equiv., (MeONMe)<sub>2</sub>C=O, to afford an intermediate ketone which is converted to the core spiroketal moiety of tautomycin upon acid treatment. Chain elongation by another addn. of the aforementioned allenylzinc reagent to a spiroketal aldehyde proceeds with high diastereoselectivity to install the remaining stereocenters. The resulting homopropargylic alc. adduct is converted to a Me ketone (I) through intramol. hydrosilylation of the alkyne and Tamao oxidn. of the derived five-membered siloxane. I proved identical to an intermediate employed by Chamberlin in a prior total synthesis of tautomycin.

RX(131) OF 502 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d ind 2

L17 ANSWER 2 OF 6 CASREACT COPYRIGHT 2002 ACS  
 CC 26-6 (Biomolecules and Their Synthetic Analogs)  
 ST tautomycin precursor asym synthesis hydrosilation alkyne oxidn siloxane  
 IT Chirality  
 (allene; in asym. synthesis of the C1-C21 subunit of tautomycin)  
 IT Oxidation  
 (catalytic, Tamao; of siloxane in asym. synthesis of the C1-C21 subunit of tautomycin)

IT Hydrosilylation  
 (intramol.; in prepn. of .beta.-hydroxy ketones during asym. synthesis of the C1-C21 subunit of tautomycin)

IT Spiro compounds  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (ketals; asym. synthesis of the C1-C21 subunit of tautomycin)

IT Asymmetric synthesis and induction  
 (of the C1-C21 subunit of tautomycin)

IT Ketals  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (spiroketals; asym. synthesis of the C1-C21 subunit of tautomycin)

IT 109946-35-2P, Tautomycin  
 RL: PNU (Preparation, unclassified); PREP (Preparation)  
 (asym. synthesis of the C1-C21 subunit of tautomycin)

IT 867-13-0 3282-30-2 6638-79-5, N,O-Dimethylhydroxylamine hydrochloride  
 15933-59-2 18618-55-8, Cerium trichloride heptahydrate 64740-39-2  
 73647-37-7 77943-39-6 81927-55-1 87727-28-4 97826-89-6  
 104701-87-3 235099-42-0 236390-96-8 289900-03-4 329914-00-3  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (asym. synthesis of the C1-C21 subunit of tautomycin)

IT 81678-44-6P 105859-49-2P 123707-26-6P 128329-72-6P 135212-08-7P  
 143728-66-9P 159563-09-4P 165961-54-6P 252235-01-1P 329913-79-3P  
 329913-80-6P 329913-81-7P 329913-82-8P 329913-83-9P 329913-85-1P  
 329913-87-3P 329913-91-9P 329913-92-0P 329913-94-2P 329913-95-3P  
 329913-97-5P 329913-98-6P 329914-01-4P 329914-03-6P 329914-05-8P  
 329914-07-0P 329914-08-1P 329914-10-5P 329914-11-6P 329914-13-8P  
 329914-15-0P 329914-16-1P 329914-17-2P 329914-18-3P 329914-19-4P  
 329914-20-7P 329914-21-8P 329914-22-9P 329914-23-0P 329914-24-1P  
 329914-25-2P 329914-26-3P 329914-27-4P 329914-29-6P 329914-30-9P  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (asym. synthesis of the C1-C21 subunit of tautomycin)

IT 185670-19-3P 329914-28-5P 329914-31-0P  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (asym. synthesis of the C1-C21 subunit of tautomycin)

=&gt; d ibib abs fcrdref 3

L17 ANSWER 3 OF 6 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 133:135044 CASREACT

TITLE: Synthesis of aromatic triynes as precursors to  
helicene derivativesAUTHOR(S): Stara, Irena G.; Kollarovic, Adrian; Teply, Filip;  
Stary, Ivo; Saman, David; Fiedler, PavelCORPORATE SOURCE: Inst. Organic Chemi. Biochem., Acad. Sci. Czech  
Republic, Prague, 166 10, Czech Rep.SOURCE: Collection of Czechoslovak Chemical Communications  
(2000), 65(4), 577-609

CODEN: CCCCAC; ISSN: 0010-0765

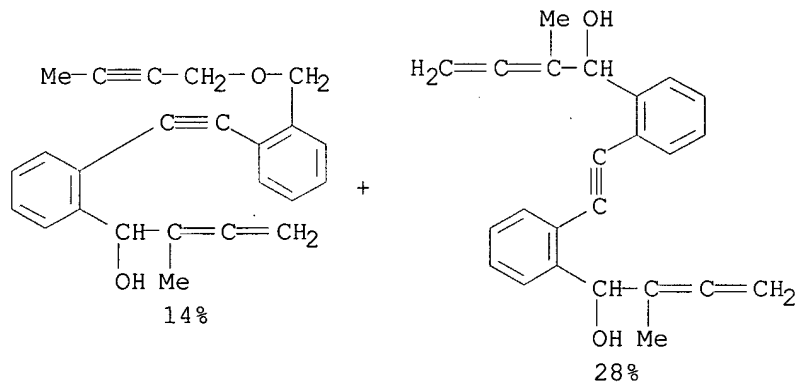
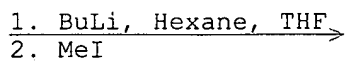
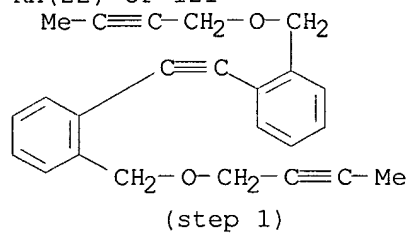
PUBLISHER: Institute of Organic Chemistry and Biochemistry,  
Academy of Sciences of the Czech Republic

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A general and versatile synthetic approach to a broad series of arom.  
triyne as precursors to helicene derivs. has been developed. Employing a  
set of simple tools, triynes comprising the (phenylethynyl)benzene,  
1-(phenylethynyl)naphthalene, and 1-(1-naphthylethynyl)naphthalene moiety  
have been prep'd. in good to excellent yields throughout the whole reaction  
sequence. The methodol. allows constructing various types of a junction  
between the central diarylacetylene moiety and the attached acetylene  
units to get the target triynes of general formula  
RC.tplbond.CCH2XCH2ArC.tplbond.CAr'CH2XCH2C.tplbond.CR or  
RC.tplbond.CCH2CH2ArC.tplbond.CAr'CH2CH2C.tplbond.CR (R = H, CH3, TMS,  
TIPS; X = O, NTs, C(CO2CH3)2; Ar/Ar' = 2-phenylene, 2-naphthylene).

RX(22) OF 121



REF: Collection of Czechoslovak Chemical Communications, 65(4), 577-609; 2000

REFERENCE COUNT:

64

THERE ARE 64 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=&gt; d ibib abs fcrdref 4

L17 ANSWER 4 OF 6 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 129:260244 CASREACT

TITLE: Chemistry of natural compounds and bioorganic chemistry synthetic research on hepoxilins. 7. Divergent total synthesis of hepoxilins and related eicosanoids

AUTHOR(S): Mel'nikova, V. I.; Vasil'eva, L. L.; Pivnifsky, K. K.

CORPORATE SOURCE: Institute of Experimental Endocrinology of the National Endocrinology Scientific Center, Russian Academy of Medical Sciences, Moscow, 115478, Russia  
SOURCE: Russian Chemical Bulletin (Translation of Izvestiya Akademii Nauk, Seriya Khimicheskaya) (1998), 47(6), 1199-1208

CODEN: RCBUEY; ISSN: 1066-5285

PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new synthetic strategy for hydroxy-epoxy eicosanoids formed through the lipoyxygenase pathway is developed. It makes use of a single synthon of the central functionalized fragment of the target mols., namely racemic (E)-ClCH2C.tplbond.CCHOHCH=CHCH2OBz. Elongation of the carbon chain of the synthon by successive condensations at both ends alternatively with hept-1-yne and hex-5-ynoic acid followed by enantioselective double bond epoxidn. and partial hydrogenation of the triple bonds resulted in the syntheses of hepoxilins B3, their potential 8-lipoyxygenase analogs, or their enantiomers; depending on the sequence of carbon chain elongations and the chirality of the epoxidn. controller used.

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

=&gt; d ind 4

L17 ANSWER 4 OF 6 CASREACT COPYRIGHT 2002 ACS

CC 26-3 (Biomolecules and Their Synthetic Analogs)

ST hepoxilin eicosanoid prepn kinetic resoln; chloroheptenyndiol monobenzoate eicosanoid synthon; benzoyloxchloroheptenyndiol eicosanoid synthon; heptyne alkylation chloroheptenyndiol monobenzoate; hexynoic acid alkylation chloroheptenyndiol monobenzoate; eicosaenetriynoate prepn stereoselective epoxidn

IT Asymmetric synthesis and induction  
Synthons

(divergent total synthesis of hepoxilins and related eicosanoids)

IT Eicosanoids

RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP (Preparation)

(hepoxilins; divergent total synthesis of hepoxilins and related eicosanoids)

IT Resolution (separation)

(kinetic; divergent total synthesis of hepoxilins and related eicosanoids)

IT Epoxidation

(stereoselective; divergent total synthesis of hepoxilins and related eicosanoids)

IT 213545-39-2P 213545-47-2P 213545-51-8P 213545-54-1P



RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)  
 (divergent total synthesis of hepoxilins and related eicosanoids)

IT 127902-31-2P 213545-27-8P 213545-29-0P 213545-35-8P 213545-43-8P  
 213545-48-3P 213545-52-9P

RL: PUR (Purification or recovery); RCT (Reactant); SPN (Synthetic  
 preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (divergent total synthesis of hepoxilins and related eicosanoids)

IT 89408-74-2P, HxB3 methyl ester 213545-40-5P 213545-41-6P  
 213545-50-7P

RL: PUR (Purification or recovery); SPN (Synthetic preparation); PREP  
 (Preparation)  
 (divergent total synthesis of hepoxilins and related eicosanoids)

IT 110-65-6, 2-Butyne-1,4-diol 624-65-7, Propargyl chloride 628-71-7,  
 1-Heptyne 77758-51-1, Methyl 5-hexynoate

RL: RCT (Reactant); RACT (Reactant or reagent)  
 (divergent total synthesis of hepoxilins and related eicosanoids)

IT 54339-95-6P, 2-Butyne-1,4-diol dibenzoate 81121-63-3P,  
 cis-2-Butene-1,4-diol monobenzoate 118017-13-3P, trans-4-(Benzoyloxy)-2-  
 butenal 118017-20-2P, 2-Butyne-1,4-diol monobenzoate 127995-26-0P  
 213545-10-9P 213545-12-1P 213545-14-3P 213545-16-5P 213545-19-8P  
 213545-20-1P 213545-21-2P 213545-22-3P 213545-23-4P 213545-24-5P  
 213545-25-6P 213545-26-7P 213545-28-9P 213545-30-3P 213545-32-5P  
 213545-34-7P 213545-36-9P 213545-45-0P 213545-49-4P 213545-53-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
 (Reactant or reagent)  
 (divergent total synthesis of hepoxilins and related eicosanoids)

IT 89461-47-2P, (10R)-HxB3 methyl ester 213545-31-4P 213545-33-6P  
 213545-38-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
 (divergent total synthesis of hepoxilins and related eicosanoids)

=&gt; d ibib abs fcrdref 5

L17 ANSWER 5 OF 6 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 112:55328 CASREACT

TITLE: Total synthesis of 12-O-benzoyl-6,7,14,15-tetradehydroleukotriene B4 methyl ester: precursor of labeled LTB4

AUTHOR(S): Pontikis, Renee; Randrianasolo, Lalatiana R.; Le Merrer, Yves; Nguyen Hoang Nam; Azerad, Robert; Depezay, Jean Claude

CORPORATE SOURCE: Lab. Chim. Biochim. Pharmacol. Toxicol., Univ. Rene Descartes, Paris, 75270, Fr.

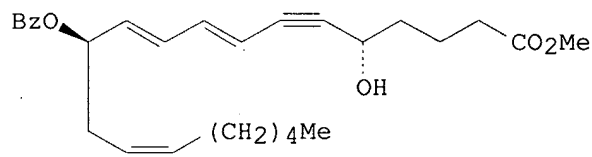
SOURCE: Can. J. Chem. (1989), 67(12), 2240-2

CODEN: CJCHAG; ISSN: 0008-4042

DOCUMENT TYPE: Journal

LANGUAGE: English

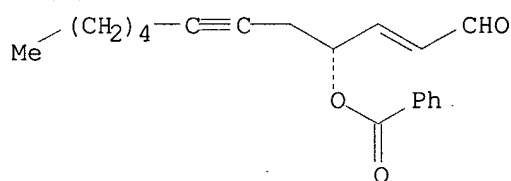
GI



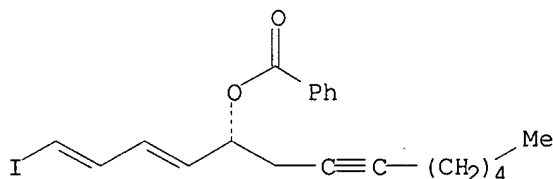
I

AB 12-O-Benzoyl-6,7,14,15-tetradehydroleukotriene B4 Me ester (I), the direct precursor of isotopically labeled LTB4, has been prepd. This synthesis was accomplished by the assembly of two key chiroins i.e. (R)-Me(CH2)4C.tplbond.CCH2CH(OBz)CHO and (S)-HC.tplbond.CCH(OH)(CH2)3CO2Me. The first was obtained from D-mannitol whereas the second was obtained by enzymic resohn.

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CrCl2, MeI, THF →



stereoisomers

70%

REF: Can. J. Chem., 67(12), 2240-2; 1989

REYES 10/088,455.

=&gt; d ibib abs fcrdref 6

L17 ANSWER 6 OF 6 CASREACT COPYRIGHT 2002 ACS

ACCESSION NUMBER: 111:77710 CASREACT

TITLE: A route to key fragments of mycotycin B and amphotericin B from (S)-O-benzylglycidol

AUTHOR(S): Takano, Seiichi; Shimazaki, Youichi; Sekiguchi, Yoshinori; Ogasawara, Kunio

CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan

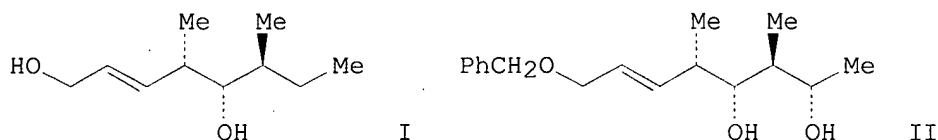
SOURCE: Chem. Lett. (1988), (12), 2041-4

CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal

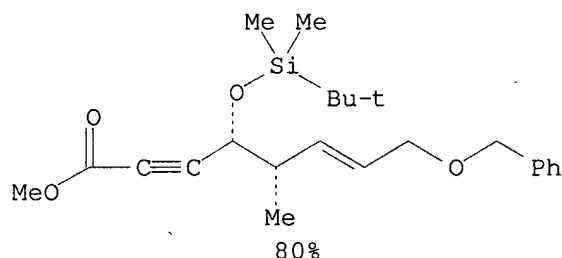
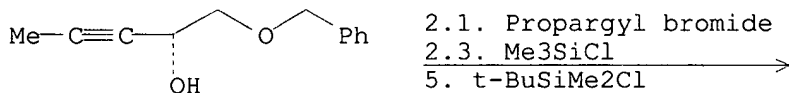
LANGUAGE: English

GI



AB A concise enantioselective synthesis of C(2)-C(34) fragment I of mycotycin B and C(31)-C(37) fragment II of amphotericin B is achieved using a common building block preps. from (S)-O-benzylglycidol.

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REF: Chem. Lett., (12), 2041-4; 1988

NOTE: 1) Lindlar catalyst